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(4) \$7.60

(5) 961 600

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(b) COMPUTER CALCULATIONS OF ROCKET
ENGINE COMBUSTION PROPERTIES,

(b) by

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- (1) NA
(2) NA
(3) NA
(4) NA
(5) NA
(6) b2P
(7) NA
(8) NA
(9) NA
(10) NA
(11) NA
(12) NA
(13) NA
(14) NA
(15) NA
(16) NA
(17) NA
(18) NA
(19) NA
(20) u
(21) Master's
thesis

A Thesis

Submitted to the Department of
Mechanical Engineering and the Graduate
School of the University of Wyoming in Partial
Fulfillment of Requirements for the Degree of
Master of Science

University of Wyoming

Laramie, Wyoming

(1) May, 1963



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ACKNOWLEDGEMENT

I can remember as a boy in Junior High School, I dreamed of being a Rocket Engineer. To the United States Air Force, to the University of Wyoming, and especially to Professor Robert A. Wheasler of the Department of Mechanical Engineering, I am deeply grateful for having the opportunity to study the subject of rocket propulsion. For the opportunity to write this paper, I will forever be in debt to all who have offered assistance.

I am also deeply indebted to the Department of Statistics for the use of the IBM 1620 Digital Computer to complete the computation which otherwise would have been impossible.

R. C. R.

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NOMENCLATURE

The following symbols are employed in the derivations of this thesis.

<u>Symbol</u>	<u>Explanation</u>
A_1	Total number of atoms of a particular species in the reactants.
a_1	The number of atoms of a particular species contained in a product of combustion.
a_j	The stoichiometric coefficient in the equilibrium equation.
(a/G)	Mole fraction of species a.
$(a/G)P$	Partial pressure of species a.
C	Centigrade temperature scale.
CONV	Convergence.
Cal	Calorie.
C_p	The value of specific heat measured at constant pressure.
C_v	The value of specific heat measured at constant volume.
CH2	C_p value for hydrogen at some T.
CH2A	C_p value for hydrogen at $T + 100$ K.
F	Fahrenheit temperature scale.
G, g	Gibb's free energy function.
G	Total number of moles when used in the equations of combustion.
gmole	Gram mole.
H, h	Enthalpy.
H_f	Heat of formation (chemical).
H_r	Heat of reaction (chemical).
H2	Enthalpy of hydrogen at T.

NOMENCLATURE (continued)

<u>Symbol</u>	<u>Explanation</u>
H _{2A}	Enthalpy of hydrogen at T + 100 K.
H _{2S}	Enthalpy of hydrogen at 298.16 K.
K	Kelvin temperature scale.
Kcal	One thousand calories.
K _p	Equilibrium constant based on partial pressure.
k	Isentropic exponent (C _p /C _v).
L	Work other than expansion work.
Log	Naperian logarithm.
M	Molecular weight.
m	Mass.
N	Number of moles.
n ₁	The number of moles of a product of combustion.
O/F	Oxidizer/fuel molar ratio.
P, p	Pressure.
P _S	Combustion pressure (atmospheres).
P _{KL}	Logarithm value of K _{PL} at some T.
P _{KLA}	Logarithm value of K _{PL} at T + 100 K.
Q	Thermodynamic heat.
R _u	Universal gas constant (1.98718 $\frac{\text{Cal}}{\text{gmole}\cdot\text{K}}$).
R _S	Fractional value between hundreds of degrees.
S, s	Entropy.
s	Molar ratio (oxidizer/fuel).

NOMENCLATURE (continued)

<u>Symbol</u>	<u>Explanation</u>
T, t	Temperature degrees absolute.
Tc	Adiabatic flame temperature.
TOLER	Tolerance level for the matrix solution.
U, u	Thermodynamic enternal energy.
V, v	Volume.
X _i	Error function of substance i.
(3,7)	(Row 3, Column 7) of the matrix.
(2:148)	(Reference 2: Page 148)

CHAPTER I
INTRODUCTION

A rocket engine is a device for converting the thermochemical energy of one or more propellants into exhaust jet kinetic energy. The term propellant is applied to any material, solid or liquid, consumed in the rocket motor for producing high-pressure, high-temperature gases. It is generally assumed, and there is some evidence to support the assumption, that, under the pressure and temperature occurring in a rocket-motor combustion chamber and nozzle, the chemical reaction takes place under conditions which approach chemical equilibrium. Accordingly, in the ensuing discussions the thermodynamic properties of the gas flowing through the rocket motor are assumed to be those from thermochemical equilibrium calculations.

(1:426)*

↓
The scope of this paper will be limited to the equilibrium calculations of combustion products and the resulting adiabatic flame temperature. The problem of attempting to determine the equilibrium constituents as the gases progress through the rocket nozzle will not be attempted at this time although this author realizes the very pronounced problem which exists. Job 2

As the static temperature decreases during the systematical progression of the gases through the nozzle, the molecules of the propellant which have dissociated due to the high temperature in the combustion chamber tend to reassociate. In a basic rocketry problem frozen flow is assumed, that is, the equilibrium combustion of the

* Numbers in parentheses refer to items in the bibliography and the related page number.

gases in the combustion chamber is unaltered during the expansion process in the nozzle. (1:436) In the condition of equilibrium flow the equilibrium composition corresponding to the local conditions of pressure and temperature is obtained in each section of the nozzle. The preceding statements correspond to the two extreme cases of frozen or equilibrium flow. In the case of real flow, at a temperature often exceeding 3000 K near the chamber, reactions of recombination take place. (2:179) However, the residence time in the nozzle is very small and these reactions may not have sufficient time for completion. Equilibrium flow, therefore, is not obtained and the real flow is situated at some intermediate point between the two extreme cases.

Before the age of electronic computers, the problem of calculating the combustion properties of a rocket engine was very tedious and almost impossible to solve. Since the present day engineers have access to the electronic computers, it is only fitting that a thesis be presented in a form illustrating the solution of combustion problems by use of the electronic computers.

The following presentation is a solution of a relatively simple combustion problem consisting of only six products of combustion. By simply understanding and following the illustrated procedures a problem consisting of any number of products of combustion may be computed and solved to any desired degree of accuracy.

CHAPTER II

HEAT OF REACTION (ΔH_r)

The energy released or absorbed in a chemical reaction, under the condition that the products are returned to the initial temperature of the reactants, is defined as the Heat of Reaction. If the reaction takes place at constant pressure, the heat of reaction is equal to the change in enthalpy during the reaction, i.e., (H) products - (H) reactants. Of course, these enthalpy values must include the energy associated with the chemical bonds of each substance as well as its thermal energy which is due to the random motion of the molecules. (4:1)

The heat of reaction at constant pressure is related to the heat of reaction at constant volume by the following thermodynamic relationships

$$dq = du + pdv = dh - vdp = dH_r \quad (1)$$

The internal energy (U) for an ideal gas is a function of temperature only. From this fact it is possible to make the assumption that for an ideal gas, the finite difference of internal energy (ΔU) at constant pressure is equal to the same value at constant volume, which defines

$$(\Delta U)_p = (\Delta U)_v \quad (2)$$

However

$$(\Delta H_r)_v = \Delta U + \cancel{\Delta P^0} \quad (3)$$

and

$$(\Delta H_r)_p = \Delta H - \cancel{\Delta P^0} \quad (4)$$

Since by definition

$$H = U + PV \quad (5)$$

then

$$\Delta H = \Delta U + \Delta(PV) \quad (6)$$

on rearranging

$$\Delta U = \Delta H - \Delta(PV) \quad (7)$$

Then by substitution

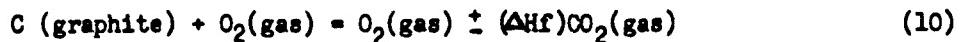
$$(\Delta H_r)_v = (\Delta H_r)_p - \Delta(PV) = (\Delta U)_p - (\Delta U)_v \quad (8)$$

which can be written as

$$(\Delta H_r)_v = (\Delta H_r)_p - (\Delta N_{\text{gas}}) R u T \quad (9)$$

Standard Heat of Formation is the heat of reaction when a compound is formed from its elements in their standard state. The standard state of an element is its stable form at a temperature of 298.16 K or 25 C and a pressure of one atmosphere. The standard state is sometimes referred to as being 0 C and one atmosphere. The standard-state temperature is really artificial, for, if the reaction were to take place isothermally, it would require a perfect heat sink which removes heat from the system as fast as it is liberated by the chemical reaction.

When a substance is combined with oxygen the heat of reaction is called the heat of combustion since the reaction is one in which the oxygen is the oxidizer. The formation of carbon dioxide from its elements in their standard state is as follows



Here the carbon must be in the graphite state since that is the stable form of carbon at 25 C, likewise the oxygen and the carbon dioxide must be in the gaseous state. Under these conditions the heat of reaction is the standard heat of formation of CO₂. In this case

the heat of reaction can also be called the heat of combustion.

The sign associated with the heat of reaction is an indication as to whether the reaction is endothermic (takes up heat) or exothermic (gives off heat). In this country normally a minus or negative sign is associated with an exothermic reaction. This convention is not true all over the world. An easy way to determine which convention is used for any particular set of tables is to check the heat of formation of water. Water will always have an exothermic heat of formation and from this, the correct sign convention can be determined for the remaining substances.

CHAPTER III

CHEMICAL EQUILIBRIUM AND THE EQUILIBRIUM CONSTANT

There are several different ways of defining and expressing the equilibrium constant. For example, depending upon the circumstances, the equilibrium constant can be based on concentrations, activities, fugacities, or partial pressures of the constituents present in the equilibrium mixture. In situations where the perfect gas law is closely followed by the constituents of the mixture, the equilibrium constant based on partial pressures is the most useful, i.e., the most easily applied.

An arbitrary thermodynamical system which is separated from its surroundings by a control surface which is a perfect thermal insulator, will now be considered. It is desired to determine from the thermodynamic characteristics of the system whether or not the system is in equilibrium or undergoing a spontaneous change of state. As a first step in the consideration of the aforementioned problem, it is necessary to determine what information can be derived by applying the first and second laws of thermodynamics to the system. The only information furnished by the first law is that one type of energy can be converted into another, and the ratio of the conversion is constant. The first law gives no information regarding the direction in which an energy transformation will proceed. As far as the first law is concerned, it is possible for the conversion to proceed in any direction that is permitted by the constraints imposed on the thermodynamic system. Thus the first law gives no information whatsoever regarding either the spontaneity or the

direction of a physical or chemical process. (2:529)

The second law established the principle that it is impossible to take heat from a system and convert it into work without simultaneous changes occurring in the system or in its environment. From the second law it is learned that only for a reversible adiabatic (isentropic) process is the entropy constant. From the entropy principle it is deduced that the only changes of state (processes) that are possible are those which produce an increase in the entropy of an isolated system. The second law gives no information indicating whether or not a process will take place if the constraints imposed on the system do allow the entropy of the system to increase. Thus it is seen that neither the first nor the second law provides the information for determining (1) whether a thermodynamic system is in equilibrium, and (2) if a spontaneous change of state can occur in a thermodynamic system.

The internal energy (U) of a thermodynamic system is analogous to the potential energy of a dynamic system. A dynamical system which is at rest can be set into motion spontaneously if the constraints imposed on it permit the potential energy of the system to diminish. The potential energy of the system tends to convert itself spontaneously into kinetic energy. Studies show that, assuming conditions permit, a dynamical system will be in equilibrium when its potential energy is a minimum. It is a fundamental principle of dynamics that a dynamical system tends to attain the state where its potential energy is a minimum, subject, of course, to the geometrical constraints imposed on the system. Thus, the internal energy (U) of a thermodynamical system, if permitted to do so, will be transformed into other forms of energy

having a nonpotential energy nature, until the equilibrium condition for the system is attained. Hence, a spontaneous change of state can take place in a thermodynamic system only if it occurs in the direction which tends to make the internal energy of the system a minimum, and the system will not be in equilibrium until the minimum value of U is attained. Hence, one fundamental principle that gives spontaneity of a process is that the process must proceed in the direction that will result in the U of the system proceeding to a condition of $U\text{-min}$.

From the second law the change of state for an isolated thermodynamic system must result in an increase in the entropy of the system. Since the entropy of the system must increase, the equilibrium condition will be attained only when no further increase in entropy is possible, that is, when the entropy of the system is a maximum, subject to the constraints imposed on it. Hence, a natural process can proceed only in the direction allowing S of the system to approach $S\text{-max}$.

From the preceding it follows that the necessary and sufficient conditions for a thermodynamical system to be in equilibrium are: (1) its internal energy must be a minimum, and (2) its entropy must be a maximum. Hence, a spontaneous process is possible only if the change of state can proceed so that the conditions of $U \rightarrow U\text{-min}$ and $S \rightarrow S\text{-max}$ are satisfied.

The free-energy denoted by G (Gibbs Function) is defined by

$$G = H - TS = U - TS + PV \quad (11)$$

Since H , U , T , and S are thermodynamic point properties, the free-energy function G is likewise a point property. Hence, a finite change, such as ΔG depends only on the final and initial states of the system.

The exact differential dg is given by

$$dg = du - tds - sdt + pdv + vdp \quad (12)$$

Combining the first and the second laws of thermodynamics results in the following familiar equations

$$tds = dq = du + pdv = dh - vdp \quad (13)$$

One very important statement which is quite often overlooked by the student of thermodynamics is that these equations are based on a pure substance, that is, a substance which is chemically homogeneous and fixed in chemical composition. If the state of the system is such that no chemical reaction can occur without an external stimulus, then the system is in complete (mechanical, thermal, and chemical) equilibrium. When in such a state, the system is chemically homogeneous and invariant; so it is a pure substance and the preceding relationships will apply. However, when a spontaneous chemical reaction occurs it is an irreversible process of a nonpure substance and the equations become (6:482)

$$tds > du + pdv \quad (14)$$

or

$$tds > dh - vdp \quad (15)$$

In the statement of the first law for a closed system, where

$$du = dq - dw \quad (16)$$

it is considered that dw is equal to $pdv + dL$, and defines dL as work other than expansion work; the tds equations for a chemical reaction may then be written as

$$tds = du + pdv + dL \quad (17)$$

or

$$tds = dh - vdp + dL \quad (18)$$

The free-energy equation is then stated as

$$dg = du + pdv + vdp - tds - sdt \quad (19)$$

Then substituting for tds from equation (17)

$$dg = du + pdv + vdp - (du + pdv + dL) - sdt \quad (20)$$

which results in

$$dg = vdp - sdt - dL \quad (21)$$

In the special case where $dp = 0$ and $dt = 0$, the finite change in free-energy for such a process is denoted by

$$(\Delta G)_{tp} = (G_2 - G_1)_{tp} = -\Delta L \quad (22)$$

This equation shows that the change in the free-energy function $(\Delta G)_{tp}$ represents the maximum (nonexpansion) useful work obtained from a constant temperature and pressure process. It also shows that, for a process conducted so that $dp = 0$ and $dt = 0$, the useful work ΔL is equal to the decrease in the value of the free-energy function.

The free-energy function finds its principal use in establishing the criteria for predicting the equilibrium of chemical and physical processes. For a system that is in equilibrium at a given temperature and pressure, the value of the free-energy function is a minimum. Moreover, for a process to take place spontaneously without change in temperature and pressure, the corresponding change in the free-energy function must be negative. Hence, for a spontaneous change (with $dp = 0$ and $dt = 0$)

$$(\Delta G)_{tp} = (G_2 - G_1)_{tp} < 0 \quad (23)$$

The foregoing provides a criterion for the possible existence of equilibrium. If $(\Delta G)_{tp} = 0$, a spontaneous change of state is impossible. The foregoing shows that, if the free-energy function at a second state (state 2) is less than it is in the initial state (state 1), the system must eventually pass to state 2. Thus the change in the free-energy function is a measure of the tendency of a system to change its state; that tendency is called the escaping tendency.

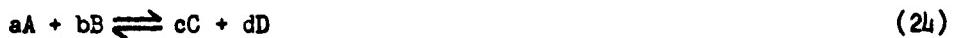
From the discussion of the free-energy function the following conclusions may be drawn.

1. The only chemical reaction that can proceed spontaneously are those for which the free-energy function decreases.
2. If a chemical reaction gives no change in the free-energy function, then the reaction is in the equilibrium state.
3. Since the direction of a chemical reaction depends on the concentrations of the chemical species involved, the values of the free-energy function for the different species are related to their concentrations.
4. If the reactants in a chemical process cannot form the desired products by a given isothermal process, they cannot form them by any other process, because the change in the free-energy function is independent of the path since it is a property.

When H_2O and CO_2 and other products of combustion are subject to temperatures of 4300 F and higher they tend to dissociate in a manner and to a degree determined solely by the temperature of the mixture. When the products of combustion dissociate, heat is absorbed, which decrease the energy available to accelerate the combustion gases

through the rocket engine. Dissociation is a reversible reaction, that is, one that will go in either direction. In any mixture of products and reactants both dissociation and combustion are constantly occurring. When the rate of dissociation equals the rate of combustion the reaction is in chemical equilibrium and an equilibrium constant exists.

In the general chemical reaction



A, B, C, D represent various substances and a, b, c, d represent the corresponding stoichiometric coefficients. (9:498)

For this example it will be assumed that all the substances involved represent ideal gases. The double arrow indicates that when equilibrium is achieved each substance will be present in a certain amount, and each substance will exist at its partial pressure. As previously stated for a system to be in equilibrium dL must equal 0, that is, no work is being done. From this, equation (21) becomes

$$dg = vdp - sdt \quad (25)$$

which for a isothermal process reduces to

$$dg = vdp = \frac{R_u T}{p} dp \quad (26)$$

Then upon intergrating from p^0 to p and g^0 to g , equation (26) becomes

$$g - g^0 = R_u T \log \frac{p}{p^0} \quad (27)$$

By letting subscript zero refer to standard conditions at one atmosphere

$$g - g^0 = R_u T \log p \quad (28)$$

where p is in atmospheres.

From the mixture of gases as given in the previous general

equation (24), the following can be written

$$g_A - g_A^{\circ} = R_u T \log p_A \quad (29)$$

$$g_B - g_B^{\circ} = R_u T \log p_B \quad (30)$$

$$g_C - g_C^{\circ} = R_u T \log p_C \quad (31)$$

$$g_D - g_D^{\circ} = R_u T \log p_D \quad (32)$$

Now by writing an expression for the change in Gibb's free-energy function as the reaction goes to completion, that is, starting with reactants A and B and ending with products C and D and since

$$\Delta G = G_{\text{products}} - G_{\text{reactants}} \quad (33)$$

then

$$\Delta G = cg_C + dg_D - ag_A - bg_B \quad (34)$$

Substitution in the pressure equations (29) through (32), gives

$$\Delta G = cg_C^{\circ} + c R_u T \log p_C + dg_D^{\circ} + d R_u T \log p_D$$

$$-ag_A^{\circ} - a R_u T \log p_A - bg_B^{\circ} - b R_u T \log p_B \quad (35)$$

However, ΔG° is defined as

$$\Delta G^{\circ} = cg_C^{\circ} + dg_D^{\circ} - ag_A^{\circ} - bg_B^{\circ} \quad (36)$$

and equation (35) then reduces to

$$\Delta G = \Delta G^{\circ} + R_u T \log \frac{p_C^c p_D^d}{p_A^a p_B^b} \quad (37)$$

When the reaction is in equilibrium ($\Delta G = 0$), and since ΔG° is a constant and $R_u T$ is a constant, the quantity

$$\log \frac{P_C^c P_D^d}{P_A^a P_B^b} \quad (38)$$

must be equal to a constant which is defined as

$$\log K_p \quad (39)$$

This results in the following equality

$$K_p = e^{-\frac{\Delta G^\circ}{RT}} \quad (40)$$

where K_p is the equilibrium constant expressed by the partial pressures of the combustion gases.

For this paper no attempt will be made to consider the equilibrium constant which is expressed in values of concentrations, activities, or fugacities.

CHAPTER IV

CALCULATION OF THE ADIABATIC FLAME TEMPERATURE

All methods for determination of the adiabatic flame temperature and the composition of the combustion products are based on two principles: the First Law of Thermodynamics and the Law of Conservation of Mass. These two principles when used in conjunction with experimentally determined chemical equilibrium data, yield a system of simultaneous equations in terms of the gas composition. The various methods of determining the gas composition differ in the manner in which the simultaneous equations are set up and solved.

By applying the First Law of Thermodynamics and the Law of Conservation of Mass to a chemical reaction it is possible to define the term Adiabatic Flame Temperature. Assuming that the chemical reaction is at constant pressure and adiabatic, and that there is no shaft work performed, the First Law of Thermodynamics states that the enthalpy of the reactants at their temperature prior to the reaction (T_b) is equal to the enthalpy of the products of the reaction at the flame temperature (T_c). Here the enthalpy must include the chemical energy of the molecules of each species as well as their energy due to random motion, since changes in internal energy occur as a result of the rearrangement of the molecules during reaction.

The Law of Conservation of Mass applied to a chemical reaction requires that the number of atoms of each element remain constant. For example, the number of atoms of a single element in the products after the reaction must be equal to the number of atoms of the same element

in the reactants prior to the reaction, and the same is true for all other elements. Thus in accordance with the definition of a mole, it can be said that the number of atoms of any particular species is constant.

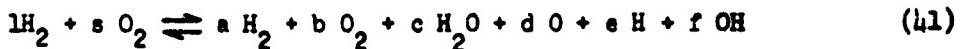
With the aforementioned laws of natural response, the necessary equations and calculations may now be presented for solving any possible system of combustion. For this combustion problem liquid hydrogen and liquid oxygen will be burned. However, by simply rearranging some of the basic steps, any oxidizer - fuel combination, may be used.

Now before the reaction equations can be written, a decision must be made as to what products of combustion are likely to be present in the combustion gas. For the adiabatic reaction, the equilibrium flame temperature will be very high and a considerable amount of dissociation can be expected.

A basic knowledge of chemistry is required to determine the possible products. By comparing the equilibrium constants of the selected products, some may be eliminated by observing that their K_p value is several orders of magnitude less than the values listed for the other reactions. The presence of other combinations may be discounted when the experimental fact is considered that a chemical system will tend to adjust itself so that the constituents are in their lowest energy state. After a decision has been reached with regard to the products of combustion, the reaction equations can then be written.

In the combustion of liquid oxygen and liquid hydrogen, a possible assumption of probable products are, H_2 , O_2 , H_2O , O , H , OH , O_3 , and H_2O_2 . O_3 and H_2O_2 can be eliminated by applying the above-mentioned rules as these are both high energy forms.

The following equation



list the six assumed products of combustion. The value of s/l will give the molar, oxidizer to fuel ratio. This can easily be converted to mass ratio, if desired, by use of the following equation

$$m = N M \quad (42)$$

However, for this problem only the molar ratio will be considered.

In the development of the system for solving for the molar values of the products of combustion it is necessary to regress a moment to discuss the selected system. "The errors are distributed among all the species" is the title of reference (2:142). This method is completely general and can be used irrespective of the number of substances present in the combustion products. The system is well suited for solution by electronic computers, which is the primary reason it was selected.

The system of equations used to determine the equilibrium composition at a given pressure and temperature is formed by linear equations representing the conservation of the species and by non-linear equations which can be written in logarithmic form and represent the various equilibria.

By referring to equation (41) and utilizing the basic equation for the balance of individual species

$$A_1 = \sum_i n_i \quad (43)$$

the first three equations may be formed.

1. Equation for hydrogen balance

$$2 = 2a + 2c + e + f \quad (44)$$

2. Equation for oxygen balance

$$2s = 2b + c + d + f \quad (45)$$

3. Equation for total moles

$$G = a + b + c + d + e + f \quad (46)$$

For any combustion problem, the number of products of combustion is equal to I, and the number of different species (atoms) is equal to J. Then from the equation

$$Y = I - J \quad (47)$$

the value of Y will determine the absolute number of independent equilibrium equations.

For this problem

$$Y = 6 - 2 \quad (48)$$

or

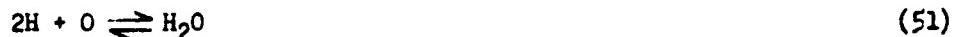
$$Y = 4 \quad (49)$$

Therefore, the number of independent equilibrium equations is 4. The basic equation for equilibrium in logarithmic form is

$$\log z_1 = \sum_{ij} a_j \log n_i \quad (50)$$

which allows the formation of the following four additional equations.

The values of K_p listed in NACA Report 1037 and also in the Appendix are based on the constituents being formed from their atoms. Therefore, the equations become

4. H_2O Equilibrium Equation, which is formed from

and results in

$$K_p(H_2O) = \frac{((c/G)p)}{((e/G)p)^2 (d/G)p} \quad (52)$$

which by rearranging becomes

$$K_p(H_2O) = \frac{c}{e^2 d} \frac{G^2}{P^2} \quad (53)$$

Then by equating

$$K_p(H_2O) = K_{p1} \quad (54)$$

In logarithmic form equation (53) may be stated as

$$2 \log P + \log K_{p1} = \log c - 2 \log e - \log d + 2 \log G \quad (55)$$

5. H_2 Equilibrium Equation, which is formed from



and results in

$$K_p(H_2) = \frac{(a/G)P}{((e/G)P)^2} \quad (57)$$

which by rearranging becomes

$$K_p(H_2) = \frac{a}{e^2} \frac{G}{P} \quad (58)$$

Then by defining $K_p(H_2)$ as K_{p2} and writing in logarithmic form, equation (58) may be stated as

$$\log P + \log K_{p2} = \log a - 2 \log e + \log G \quad (59)$$

6. OH Equilibrium Equation, which is formed from



and results in

$$K_p(OH) = \frac{(f/G)P}{(d/G)P (e/G)P} \quad (61)$$

which by rearranging becomes

$$K_p(OH) = \frac{f}{de} \frac{G}{P} \quad (62)$$

Then by defining $K_p(OH)$ as K_p3 and writing in logarithmic form, equation (61) may be stated as

$$\log P + \log K_p3 = \log f - \log d - \log e + \log G \quad (63)$$

7. O_2 Equilibrium Equation, which is formed from



and results in

$$K_p(O_2) = \frac{(b/G)_p}{((d/G)p)^2} \quad (65)$$

which by rearranging becomes

$$K_p(O_2) = \frac{b}{d^2} \frac{G}{P} \quad (66)$$

Then by defining $K_p(O_2)$ as K_p4 and writing in logarithmic form, equation (65) may be stated as

$$\log P + \log K_p4 = \log b - 2 \log d + \log G \quad (67)$$

This results in an array of mathematical logic consisting of seven equations and seven unknowns. Such a system can be solved by trial and error. It can be linearized by choosing arbitrary values for the number of moles (n_i^0) and then solving for an error function (X_i^0). The error functions are used in the following equation

$$n_i = n_i^0 (1 + X_i^0) \quad (68)$$

If X_i^0 is sufficiently small, equation (68) in logarithmic form may be written as

$$\log n_i \approx \log n_i^0 + X_i^0 \quad (69)$$

This is true by considering the fact that the $\log(1 + \text{small number})$ is approximately equal to the small number.

Equations (43), (44), (45), and (46) can thus be written in

the form

$$\sum_i a_i n_i^o X_i^o = A_1 - \sum_i a_i n_i^o = A_1 - A_1^o \quad (70)$$

where

$$A_1^o = \sum_i a_i n_i^o \quad (71)$$

Equations (55), (59), (63), and (67) can be written in the form

$$\sum_{ij} a_j X_i^o = \log z_1 - \sum_{ij} a_j \log n_i^o = \log \frac{z_1}{z_1^o} \quad (72)$$

where

$$\log z_1^o = - \sum_{ij} a_j \log n_i^o \quad (73)$$

The transformation of the variables is now complete. The new system is linear with respect to the error function (X_i) and can thus be solved by any standard method of solving simultaneous linear equations. The selected method is well suited for solution by electronic computers.

A complete description for the selected method to solve simultaneous linear equations is presented in the Appendix. The program is a partial replica of a method listed in the IBM listing of selected programs for the 1620 computer. (5.0.007) The original program was based on the original FORTRAN system and had to be completely rewritten so as to be suitable for use with the present FORTRAN program.

Table I, on the following page, consists of the seven linear equations of combustion consolidated into a matrix form. A detailed example is attached to Table I. It is available for additional reference, as required, to complete the formation of a similar system of equations necessary to solve other combustion problems.

TABLE I
COMBUSTION PROBLEM IN MATRIX FORM

H	1.	2.	3.	4.	5.	6.	7.	
H ₂	0 ²	H ₂ ⁰	c ²	d ⁰	e ⁰	f ⁰	g ⁰	
a								
b								
c								
d								
e								
f								
g								
1. Bal.	2a XA	0 XB	2c XC	0 XD	eXE fXF	0 XG	-	2 - (2a + 2c + e + f) = A1
0								
2. Bal.	0 XA	2b XB	c XC	d XD	0 XE fXF	0 XG	-	2S - (2b + c + d + f) = A2
N								
3. Total	a XA	b XB	c XC	d XD	eXE fXF	-cXH	XO	G - (a + b + c + d + e + f) = A3
4.	0 XA	0 XB 1 XC	-1 XD	-2 XE 0 XF	+2 XG	= 2log p + Pk1	- (log c - 2log e - log d + 2log G) = A4	
5.	1 XA	0 XB 0 XC	0 XD	-2 XE 0 XF	+1 XG	= log p + Pk2	- (log a - 2log e + log G) = A5	
6.	0 XA	0 XB 0 XC	-1 XD	-1 XE 1 XF	+1 XG	= log p + Pk3	- (log f - log e - log d + log G) = A6	
7.	0 XA +1 XB 0 XC	-2 XD	0 XE 0 XF	+1 XG	= log p + Pk4	- (log b - 2log d + log G) = A7		

The following examples illustrate how the above matrix is set up:

$$A_1 = \sum_{i,j} a_{ij} n_i \quad \text{** } n_i = n^0(1 + X_i) \quad \text{** } a_i n_i^0 = A_1 - \sum_j a_{ij} n_j^0$$

$$\begin{aligned} 2 = & 2a + 2c + e + f = 2a^0 + 2s^0 XA + 2c^0 + 2e^0 XC + e^0 + e^0 XE + f^0 + f^0 XF \\ 2s^0 XA + 2c^0 XC + e^0 XE + f^0 XF = & 2 - (2a^0 + 2c^0 + e^0 + f^0) \end{aligned}$$

$$\begin{aligned} \log z_1 = & \sum_{i,j} a_{ij} \log n_i \quad \text{** } \log n_i = \log n_i^0 + X_i \quad \text{** } \sum_{i,j} a_{ij} X_i = \log z_1 - \sum_{i,j} a_{ij} \log n_i^0 \\ 2 \log P + Pk1 = & \log c - 2 \log e - \log d + 2 \log G \\ 2 \log P + Pk1 = & \log c^0 + XC - 2 \log e^0 - 2 XE - \log d^0 - XD + 2 \log G^0 + 2 \log G \\ XC - 2 XE - XD + 2 XG = & 2 \log P + Pk1 - (\log c^0 - 2 \log e^0 - 10g d^0 + 2 \log G^0) \end{aligned}$$

The value of X_1 obtained from the solution of the matrix provides the new value of n_1^1 which is computed, for the second approximation, from the equation

$$n_1^1 = n_1^0 (1 + X_1) \quad (74)$$

A very important consideration is that the first approximation may not be very close to the correct value. It is probable that during the first few trials a value for X_1 of less than -1.00 may be computed. The program will not accept a value for X_1 of -1.00 or less; a value greater than -1.00 must then be used. In this problem -0.995 was utilized for such cases with complete success. After the assumed values are within the correct range a value of less than -1.00 will never be calculated and the calculated values of X_1 may be used completely. At this time the computer may be set to compute continuously until the desired convergence is obtained.

When the calculated error functions have a value of equal to or less than -1.00 and are then used in equation (74), a negative or zero value is calculated for n_1 . This creates errors in the calculation resulting from the computer attempting to take the log of a negative or zero number. By inserting -0.995, a very small positive value of n_1 is calculated. This answer is approximately correct since it would be impossible to actually have a negative value of a constituent.

The initial selected values for the number of moles of the products of combustion are completely arbitrary; however, if any information on the approximate values is available, it should be utilized. After the problem is solved one time it is advisable to use the calculated values

as the original selected values for the number of moles in solving the problem for the new temperature selection as determined by Figure 4-1. This will allow the problem to converge quicker and save having to replace the error functions that are equal to or less than -1.00. Another suggestion is to require the sum of the first selected values not to exceed the value of the number of moles of the reactants.

The convergence of the system is given by the expression

$$\text{CONV} = /A_1 - A_1^0/ + /...../ + / \ln \frac{z_1}{z_1^0} / + /.....? \quad (75)$$

In the computer program, the value of $A_1 - A_1^0$ is set equal to A_1 and the value of the $\log \frac{z_1}{z_1^0}$ is set equal to A_4 . By reference to the initial equations (44) and (55), it is quite apparent that when the correct values for the number of moles of the products have been computed A_1 , A_2 , A_3 , A_4 , A_5 , A_6 , and A_7 will all be equal to zero.

When the computer does not have the ability to add absolute values, a simple method that may be used calls for adding the sum of $\sqrt{x \cdot x}$. The system is solved when the value of C becomes sufficiently small.

The method described above will now be applied in the solution of a problem involving the selected propellants of liquid oxygen and liquid hydrogen.

The K_p values listed in NACA 1037 are presented in logarithmic form to the base 10. The logarithmic program on the 1620 computer is based on the Naperian Logarithm Scale. To be consistent the values for K_p are multiplied by the natural logarithm of 10.

The computer program is subdivided into four parts:

1. Solution of the coefficients and the values for the solution column of the matrix.

2. Assignment of the appropriate values to columns and rows of the matrix program.

3. Solution of the matrix program.

4. Solution of the difference in enthalpies.

The value for the total number of moles has been assigned to G and GH in the computer program. The matrix coefficient (GH) in position (3, 7) of the developed matrix created some confusion, during the early stages of the problem. By experimentation it was found that by letting GH be equal to the new value for the total number of moles calculated from the value of XG and by letting the G equal the sum of the new values for the n_i 's the problem would converge. However, by reversing the value of G and GH the problem would not converge.

The computer program is designed to automatically replace any undesired error function with -0.995. This ability is dependent on the position of Sense Switch 3 which also controls the type out of solutions. When Sense Switch 3 is in the off position all values are typed out by the typewriter. During the type-out of the solution of the error functions, if one has a value of -1.00 or less, it is changed to -0.995. A message that this step has been completed is also typed out.

When the operator desires, Sense Switch 3 may be turned on to eliminate typing of all values except the value of convergence. This also eliminates the ability to change the error functions; therefore, it is important that the convergence value must be observed to be decreasing before this step is performed. If Sense Switch 3 is turned on prematurely and an undesired value of an error function is computed, an error statement will be typed out indicating that the computer has

been requested to take the logarithm of a negative number. The solution must be restarted as all values are then incorrect.

As the convergence approaches the desired limit, Sense Switch 3 may be turned off. This allows all values to be typed out which are then the correct solutions for the number of moles of each of the products of combustion.

By turning on Sense Switch 2, the computer branches to the fourth subdivision, where the difference in enthalpies is computed.

The computer also has been programed to interpolate linearly, as necessary, all values of input data. The value of RS is the fractional value between hundreds of degrees. If it is desired to compute for 3528 K, values for 3500 K and 3600 K are read into the computer. The value of RS is then 0.28.

The present computer, with 20,000 storage locations, did not have sufficient locations to compute the value of the molecular weight and the isentropic exponent. A second program was written to perform this computation. The last step of the first program is the command to punch out on data cards, the solution for the number of moles of each of the products. These solution cards are then used in the second program with the necessary additional data to compute the molecular weight and the isentropic exponent. This program also has the ability to interpolate linearly the necessary data.

For the design calculations in this problem the reactants will be assumed to be at standard conditions (298.16 K). The problem is then solved for a particular molar ratio and a selected chamber or total pressure (23 atmospheres). The necessary values are taken from

NACA 1037 by assuming a particular combustion temperature. The combustion products and the change in enthalpies (ΔH) are then calculated. ΔH is defined as the enthalpy of the products taken at the combustion temperature minus the enthalpy of the reactants taken at the temperature prior to combustion. If the assumption for the combustion temperature is correct, ΔH will be equal to zero. If $\Delta H > 0$ the assumed temperature was too high; a lower value must be chosen, and combustion of the gas must be recalculated for the new temperature. Of course, if $\Delta H < 0$ then a larger value for the temperature must be selected. Repetition of this procedure two or three times will usually yield the correct value of temperature, by graphical interpolation.

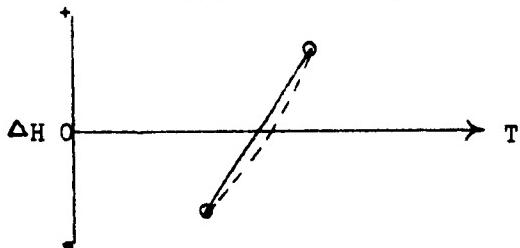


Figure 4-1. Interpolation for adiabatic flame temperature.

If the first two assumed values of temperature give values of ΔH on each side of the zero line as shown in Figure 4-1, an approximate value of the combustion temperature may be determined by linear interpolation; however, since the curve of ΔH vs T is usually concaved up, the value so determined will usually be less than the actual temperature.

Linear interpolation for the proper values of H and K_p is acceptable. It should be noted that linear interpolation for K_p over a wide temperature ranges is not accurate, and logarithmic interpolation is required for adequate approximations. However, the equilibrium constants in

NACA 1037 are tabulated for every one hundred degrees Kelvin and linear interpolation within this range of temperature yields sufficiently accurate results.

The following pages consisting of Table II and Table III have the complete computer program for liquid hydrogen and liquid oxygen. With the previous explanations and a basic knowledge of the IBM 1620 FORTRAN system, no problem should exist in setting up the program to compute the combustion properties for any propellant combination.

TABLE II

FIRST COMPUTER PROGRAM

```

DIMENSION X(7,8)
81 FORMAT(//(F12.8))
32 FORMAT(//8HSOLUTION)
33 FORMAT(44HDIAGONAL THAT IS LESS THAN OR EQUAL TO TOLER)
34 FORMAT(2HIS I3)
40 FORMAT(E11.8)
READ 40, PK1,PK2,PK3,PK4,PS,S,TOLER,RS
READ 40,PK1A,PK2A,PK3A,PK4A
READ 40,A,B,C,D,E,F
READ 40,XA,XB,XC,XD,XE,XF,XG
PK1=PK1 - RS*(PK1 - PK1A)
PK2=PK2 - RS*(PK2 - PK2A)
PK3=PK3 - RS*(PK3 - PK3A)
PK4=PK4 - RS*(PK4 - PK4A)
27 G=A+B+C+D+E+F
A=A*(1.+XA)
B=B*(1.+XB)
C=C*(1.+XC)
D=D*(1.+XD)
E=E*(1.+XE)
F=F*(1.+XF)
GH=G*(1.+XG)
G=A+B+C+D+E+F
H=LOG(10.)
A1=2.-(2.*A+2.*C+E+F)
A2=2.*S-(2.*B+C+D+F)
A3 = G-(A+B+C+D+E+F)
A4=2.*((LOG(PS))+H*PK1-(LOG(C)-2.*LOG(E)-LOG(D)+2.*LOG(G)))
A5=(LOG(PS))+H*PK2-(LOG(A)-2.*LOG(E)+LOG(G))
A6=(LOG(PS))+H*PK3-(LOG(F)-LOG(E)-LOG(D)+LOG(G))
A7=(LOG(PS))+H*PK4-(LOG(B)-2.*LOG(D)+LOG(G))
CONV=SQRT(A1*A1)+SORT(A2*A2)+SQRT(A3*A3)+SQRT(A4*A4)+SQRT(A5*A5)
CONV=CONV+SQRT(A6*A6)+SQRT(A7*A7)
IF (SENSE SWITCH 3)50,51
51 PRINT81,A1,A2,A3,A4,A5,A6,A7
PRINT 81,A,B,C,D,E,F,G,GH
50 PRINT 81,CONV
IF(SENSE SWITCH 2)30,31
31 X(1,1)=2.*A
X(2,1)=0.
X(3,1)=A
X(4,1)=0.
X(5,1)=1.
X(6,1)=0.
X(7,1)=0.
X(1,2)=0.

```

```

X(2,2)=2.*B
X(3,2)=B
X(4,2)=0.
X(5,2)=0.
X(6,2)=0.
X(7,2)=1.
X(1,3)=2.*C
X(2,3)=C
X(3,3)=C
X(4,3)=1.
X(5,3)=0.
X(6,3)=0.
X(7,3)=0.
X(1,4)=0.
X(2,4)=D
X(3,4)=D
X(4,4)=-1.
X(5,4)=0.
X(6,4)=-1.
X(7,4)=-2.
X(1,5)=E
X(2,5)=0.
X(3,5)=E
X(4,5)=-2.
X(5,5)=-2.
X(6,5)=-1.
X(7,5)=0.
X(1,6)=F
X(2,6)=F
X(3,6)=F
X(4,6)=0.
X(5,6)=0.
X(6,6)=1.
X(7,6)=0.
X(1,7)=0.
X(2,7)=0.
X(3,7)=-GH
X(4,7)=2.
X(5,7)=1.
X(6,7)=1.
X(7,7)=1.
X(1,8)=A1
X(2,8)=A2
X(3,8)=A3
X(4,8)=A4
X(5,8)=A5
X(6,8)=A6
X(7,8)=A7
N = 7
N1 = N + 1
DO 14 I = 1, N, 1

```

```

DIAG = X(I,I)
IF (DIAG) 3, 20, 4
3 IF (DIAG + TOLER) 5, 19, 19
4 IF (DIAG - TOLER) 19, 19, 5
5 DO 6 J = I, N1
6 X(I,J) = X(I,J) / DIAG
   K = 1
9 IF (K-I) 11, 13, 11
11 FELMT = X(K,I)
   DO 12 J = I, N1
12 X(K,J) = X(K,J) - FELMT * X(I,J)
13 K = K + 1
   IF (K-N) 9, 9, 14
14 CONTINUE
   IF (SENSE SWITCH 3)1,28
28 J = N1
   TYPE 32
   DO 18 I=1, N
   TYPE 40, X(I,J)
   IF (X(I,J) + 1.0) 65, 65, 18
65 X(I,J) = -.995
   TYPE 66
66 FORMAT(1I1THE ABOVE VALUE HAS BEEN CHANGED TO -.995)
18 CONTINUE
   GO TO 1
19 TYPE 33
   TYPE 34,I
   GO TO 5
20 STOP
1 XA=X(1,8)
   XB=X(2,8)
   XC=X(3,8)
   XD=X(4,8)
  XE=X(5,8)
   XF=X(6,8)
   XG=X(7,8)
   GO TO 27
30 READ 40,H2S, 02S,H2,02,H20,O,H,OH
   READ 40,H2A,O2A,H20A,OA,HA,OHA
   OH = OH + RS*(OHA - OH)
   H = H + RS*(HA - H)
   O = O + RS*(OA - O)
   H20 = H20 + RS*(H20A - H20)
   O2 = O2 + RS*(O2A - O2)
   H2 = H2 + RS*(H2A - H2)
   HTS=H2S+S*O2S
   HTC=A*H2 + B*O2 + C*H20 + D*O + E*H + F*OH
   DELH=HTC-HTS
   PRINT 41,HTC,HTS,DELH
41 FORMAT (//(E14.8))
   PUNCH 40,A,B,C,D,E,F
   STOP
   END

```

TABLE III
SECOND COMPUTER PROGRAM

```

67 FORMAT (//(35HTHE MOLECULAR WEIGHT OF THE MIX IS F10.5))
68 FORMAT(28HTHE CP VALUE FOR THE MIX IS F10.5)
69 FORMAT (23HTHE VALUE FOR CP/CV IS F10.5)
40 FORMAT(E14.8)
      READ 40,A,B,C,D,E,F,S,RS
      READ 40, CH2, CO2, CH20, CO, CH, COH
      READ 40, CH2A, CO2A, CH20A, COA, CHA, COHA
      G=A+B+C+D+E+F
      CH2 = CH2 + RS*(CH2A - CH2)
      CO2 = CO2 + RS*(CO2A - CO2)
      CH20 = CH20 + RS*(CH20A - CH20)
      CO = CO + RS*(COA - CO)
      CH = CH + RS*(CHA - CH)
      COH = COH + RS*(COHA - COH)
      CPM = CH2*A/G + CO2*B/G + CH20*C/G + CO*D/G + CH*E/G + COH*F/G
      CVM = CPM - 1.98718
      CK = CPM/CVM
      CMOL = 2.*A/G + 32.*B/G + 18.*C/G + 16.*D/G + 1.*E/G + 17.*F/G
      PRINT 67,CMOL
      PRINT 68,CPM
      PRINT 69,CK
      STOP
      END

```

CHAPTER V

RESULTS OF CALCULATIONS

The results based on a combustion pressure of 23 atmospheres are the primary concern of this report. A graph relating the flame temperature, isentropic exponent, and molecular weight of the products, to the oxidizer-fuel ratio, is presented in Figure 5-2. In addition a very interesting theory of rocketry is proven - the temperature of the gases depends primarily on the oxidizer-fuel ratio, and to a small extent on combustion pressure. The latter depends, of course, on the rate at which the propellants are being consumed and the throat area of the exhaust nozzle. The curve of the flame temperatures based on a combustion pressure of 20 atmospheres is presented for demonstration of the effect resulting from varying the combustion pressure.

The program is set up for the IBM 1620 computer as described in Chapter IV. To facilitate the calculations of the initial constants and coefficients for the matrix program, the value of zero must be read in for the error functions XA, XB, XC, XD, XE, XF, and XG. A temperature is selected for which the equilibrium constants are taken from NACA 1037. In addition to the four K_p constants, values for the molar ratio (S), combustion pressure (PS), tolerance level (TOLER), and a value for the fractional number of degrees (RS) have to be read in to the computer. The tolerance level and its use are explained in the Appendix.

Subdivision three of the first computer program, consisting of the solution of the seven linear equations, has almost entirely been taken from the program listed in the Appendix. The input section has been

deleted, since each individual position of the matrix has been identified in subdivision two. The portion evaluating a zero diagonal has been amended because the only way to adjust the rows or columns of the matrix is to rewrite the program. Care should be taken in the original writing of the computer program to prevent a zero major diagonal. Specific instructions are given in the Appendix.

A tolerance level value of 0.00001 was read in at the beginning of the program. The section permitting changing of the tolerance level was omitted from the computer program. The tolerance level in this program is not very important since the calculated values of the error functions are only used to create new assumed selections for the products of combustion. As long as the convergence continues to decrease the program is successful.

The computer program has been written to interpolate, when necessary, the input data for a selected temperature falling between hundreds of degrees. An example may be illustrated by assuming the desired temperature is 3528 K. A value for RS of 0.28 must be entered in the computer along with the appropriate input data selected at 3600 K and 3500 K. The data consisting of the four K_p constants, and the enthalpy of the constituents are taken from the NACA 1037 tables in the Appendix.

The values listed in Table IV are computed from an oxidizer/fuel molar ratio of 0.5 and with a combustion pressure of 23 atmospheres. The computation was completed for temperatures of 3400 K, 3500 K, and 3600 K. The calculated values of the moles of the products are given in Table II along with the value of ΔH computed for each of the three temperatures. These values of ΔH are plotted on the graph in Figure 5-1, and then

graphically interpolated for the temperature for which ΔH is zero. The temperature was determined to be 3528 K. The problem was then computed again for a temperature of 3528 K and the resulting ΔH was within the required accuracy. As proof, the problem was then computed at 3525 K to get an estimate of the change of ΔH per degree Kelvin. The ΔH at 3528 K was +0.06076 while the ΔH at 3525 K was -0.10568. This was sufficient proof that the temperature of 3528 K was within the experimental accuracy possible in the combustion chamber of a rocket engine.

TABLE IV

RESULTS OF CALCULATIONS
FOR O/F RATIO OF (0.5) AND 23 ATMOSPHERES

Temp. K	3400	3500	3525	3528	3600
H ₂	0.1325	0.1545	0.1602	0.1609	0.1779
O ₂	.0429	.0491	.0506	.0508	.0554
H ₂ O	.8015	.7629	.7527	.7515	.7199
O	.0183	.0257	.0279	.0281	.0354
H	.0375	.0518	.0560	.0565	.0704
OH	<u>.0944</u>	<u>.1132</u>	<u>.1182</u>	<u>.1188</u>	<u>.1338</u>
G	1.1271	1.1572	1.1656	1.1666	1.1928
ΔH	-6.5760	-1.4671	-0.1057	+0.0608	+4.2998

Since the second computer program was also written to compute a linear interpolation for necessary input data, it is only required to read into the computer Cp values for the six products of combustion at temperatures of 3600 K and 3500 K. In addition, as stated before, the

computed values taken from the first program for the number of moles, the value of S, and the value of RS have to be entered as input data into the computer. The particular values of molecular weight were permanently written into the program.

The value for the molecular weight of the mixture is computed from the following equation

$$\begin{aligned} M = & (a/G)M H_2 + (b/G)M O_2 + (c/G)M H_2O \\ & +(d/G)M O + (e/G)M H + (f/G)M OH \end{aligned} \quad (76)$$

This value, for an O/F ratio of 0.5 and a combustion pressure of 23 atmospheres, was computed as

$$M = 15.42976 \quad (77)$$

The value for Cp of the mixture is computed from the following equation

$$\begin{aligned} Cp \text{ mixture} = & (a/G)Cp H_2 + (b/G)Cp O_2 + (c/G)Cp H_2O \\ & +(d/G)Cp O + (e/G)Cp H + (f/G)Cp OH \end{aligned} \quad (78)$$

This value was determined to be

$$Cp \text{ mixture} = 11.44081 \frac{\text{Cal}}{\text{gmole-K}} \quad (79)$$

From the thermodynamic identity which relates the specific heat at constant volume (Cv) to that at constant pressure (Cp), Cv will now be computed from the equation

$$Cv = Cp - Ru \quad (80)$$

where

$$Ru = 1.98718 \frac{\text{Cal}}{\text{gmole-K}} \quad (81)$$

Then from equation (79) and (80)

$$Cv = 11.44081 - 1.98718 \quad (82)$$

or

$$C_V = 9.45363 \frac{\text{Cal}}{\text{gmole-K}} \quad (83)$$

The isentropic exponent (k) is the ratio of the specific heats and is

$$k = \frac{C_P}{C_V} \quad (84)$$

or

$$k = \frac{11.44081}{9.45363} \quad (85)$$

then

$$k = 1.21020 \quad (86)$$

Table V consists of tabulated values from the calculations at different O/F ratio while holding the combustion pressure constant at 23 atmospheres. These values were computed with the same procedures as have been illustrated for an O/F ratio of 0.5

The tabulated results of the change in adiabatic flame temperature, caused by changing the combustion pressure to 20 atmospheres, is presented in Table VI. Only the variation of the flame temperature is available in Table VI as this is the only variation of importance.

TABLE V
FINAL RESULTS OF CALCULATIONS
COMBUSTION PRESSURE 23 ATMOSPHERES

O/F Molar Ratio	0.2	0.3	0.4	0.5	0.6	0.7
Tc K	2777	3300	3492	3528	3495	3440
H ₂	0.5950	0.3942	0.2476	0.1609	0.1099	0.0788
O ₂	.0000	.0013	.0139	.0508	.1106	.1865
H ₂ O	.3979	.5679	.6830	.7515	.7961	.8270
O	.0001	.0023	.0131	.0281	.0395	.0460
H	.0121	.0486	.0627	.0565	.0448	.0345
OH	.0020	.0272	.0761	.1188	.1432	.1541
G	1.0071	1.0415	1.0964	1.1666	1.2441	1.3269
M	8.3405	11.1377	13.4985	15.4298	17.0399	18.3909
Cp g/mole-K	10.2839	11.0239	11.3384	11.4408	11.4600	11.4360
Cv	8.2967	9.0367	9.3512	9.4536	9.4728	9.4488
k	1.2395	1.2199	1.2125	1.2102	1.2098	1.2103

TABLE VI
FINAL RESULTS OF CALCULATIONS
COMBUSTION PRESSURE 20 ATMOSPHERES

O/F Molar Ratio	0.2	0.3	0.4	0.5	0.6	0.7
Tc K	2758	3280	3470	3505	3476	3411

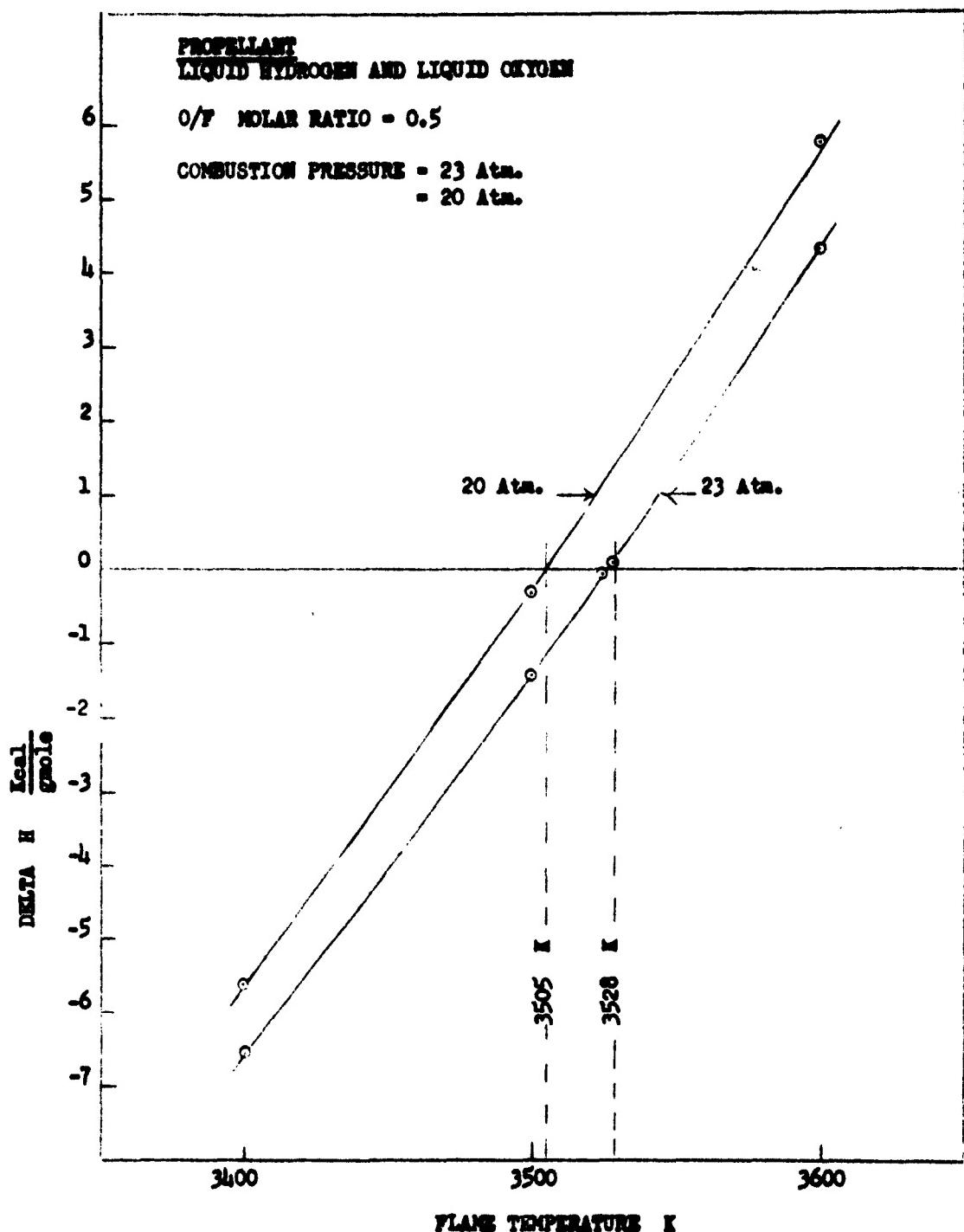


Figure 5-1. Graphical Interpolation for Combustion Flame Temperature

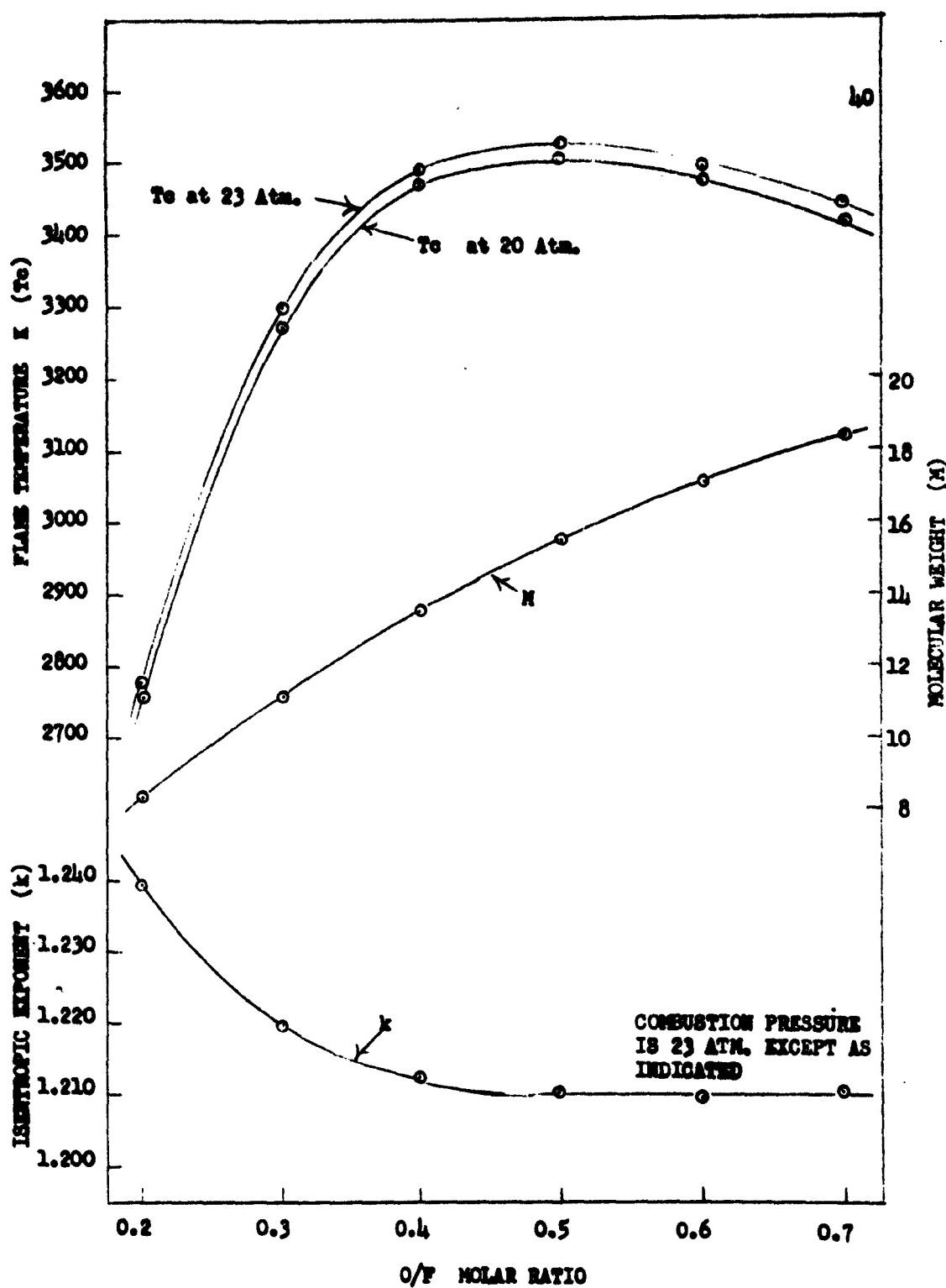


Figure 5-2. Graphical Results For Liquid Hydrogen and Liquid Oxygen

TABLE VII
RESULTS FROM FIRST PROGRAM

-.30000000 A1
-.10000000 A2
.00000000 A3
4.48435890 A4
2.05136710 A5
1.34662590 A6
1.48234660 A7

.40000000 H₂
.10000000 O₂
.40000000 H₂O
.10000000 O
.30000000 H
.40000000 OH
1.70000000 G
1.70000000 GH

9.76469830

Initial assumption
for products of
combustion.

T	3528 K
O/F	0.5
TOLER	0.00001
PS	23 Atmospheres

Initial convergence value

SOLUTION

-.52371340E-00 XA
-.43600000E-00 XB
.11604744E+01 XC
-.11695445E+01 XD
THE ABOVE VALUE HAS BEEN CHANGED TO -.995
-.14979106E+01 XE
THE ABOVE VALUE HAS BEEN CHANGED TO -.995
-.90008880E-00 XF
-.42074042E-00 XG

Results of initial calculations
for the error functions.

-.15087310
-.01745420
.00000000
-11.40451800
-7.41533000
-6.55833300
-8.15338600

.19051464
.05640000
.86418976
.00050000
.00150000
.03996448
1.15306880
.98474132

The following four pages are the
computer results from the following
input data:

33.69989100

SOLUTION

-.18793932E-00
.18042300E-02
-.75171440E-01
.40532358E+01
.35893352E+01
.11329576E+01
-.48720557E-01

-.00000020
-.00000000
.00000000
-.6.57387400
-.4.11718150
-.4.12958100

.15470945
.05650175
.79922741
.00252661
.00688400
.08524254
1.10509170
1.09689070

19.69326700

SOLUTION

.34152510E-01
-.73875990E-01
-.34020070E-01
.24102371E+01
.20865257E+01
.34546440E-00
.21717281E-01

-.00000010
-.00000010
.00000000
-.3.10104200
-.1.91799860
-.2.09381940

.15999316
.05232763
.77203769
.00861636
.02124765

.11469080
 1.12891320
 1.12909120

9.47650880

3.06712780

Here Sense Switch 3 was turned on.

.44407657

.01147719

.00000870

Here Sense Switch 3 was turned off.

SOLUTION

.38571400E-06
 -.58173300E-06
 .43619820E-07
 .15603613E-05
 .49408466E-06
 -.114800950E-06
 .10245536E-06

.00000010 A1
 -.00000000 A2
 .00000000 A3
 -.00000020 A4
 -.00000010 A5
 -.00000020 A6
 -.00000020 A7

.16086923 H₂
 .05080107 O₂
 .75149282 H₂O
 .02813721 O
 .05650815 H
 .11876787 OH
 1.16657620 G
 1.16657620 GH

.00000080

Final convergence value

.71556908E+02
 .71496150E+02
 .60758000E-01

Enthalpy of products at 3528 K
 Enthalpy of reactants at 298.16 K
 ΔH

STOP

The values of the error
 functions are now very small
 numbers.

Final values for the
 products of combustion.

TABLE VIII
RESULTS FROM SECOND PROGRAM

THE MOLECULAR WEIGHT OF THE MIX IS 15.42976
THE CP VALUE FOR THE MIX IS 11.44081
THE VALUE FOR CP/CV IS 1.21020
STOP

BIBLIOGRAPHY

BIBLIOGRAPHY

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APPENDIX

SOLUTION OF SIMULTANEOUS LINEAR EQUATIONS

Introduction

This program is a replica of program number (5.0.007) from the IBM 1620 General Program Library. It has been rewritten as necessary to be compatible with the present 1620 (20K) computer and the FORTRAN programming system with format statements. Although this program was tested by its author using the sample problems, no warranty, expressed or implied, is made by the author or IBM.

Description of the Program

A knowledge of the IBM 1620 FORTRAN system is required to understand the following program.

This program solves sets of non-homogeneous simultaneous linear equations and provides either typewriter or punched card output. Up to 25 equations in 25 unknowns may be solved. The first card read for each set of equations states the number of equations following. The program automatically sizes itself for the proper matrix dimensions. Any number of sets of equations may be solved one after the other without reloading the program deck. When a solution has been obtained the word SOLUTION is typed. Under this heading the solution variables are typed one per line in the order in which they appear from left to right in the original equations. Punched card output is identical, with one card punched for each line typed.

If a set of equations is submitted which has more than one solution, a valid solution will be typed or punched, but no indication will be given that there are other solutions as well.

If the equations in the set are not all independent, a typewriter message will indicate that a diagonal element is zero. No solution is developed in this case, as there are infinite solutions to the set of equations.

Additional information regarding the characteristics of the program is contained in the discussion of the method of computation.

Method of Computation

General Description. The Jordan method of elimination¹ is used to accomplish the solution. Briefly this method consists of diagonalizing the augmented coefficient matrix. After diagonalization the right hand or augmented column contains the solution values for the variables.

The reduction of the matrix takes place in the same storage locations where the original coefficients are stored. Thus at the completion of the solution the original coefficients are lost, and in

¹

Alston S. Householder, Principles of Numerical Analysis (New York: McGraw-Hill Book Co., Inc., 1953), pp. 68-72.

their place remain an identity matrix and the column of answers.

Division by a Zero Diagonal. In the process of diagonalization the elements of each row to the right of the diagonal and the diagonal itself are divided by the diagonal element. The diagonal elements are used in the same order in which they appear in the original matrix. No attempt is made to select these pivotal elements by magnitude. Hence a zero must not appear on the diagonal of the matrix. If such a condition exists, a message will be typed indicating which diagonal element is zero and control passes to reading the next problem.

The possibility of zero diagonal elements may be minimized by observing two rules in laying out the original matrix.

1. The upper left hand element should not be zero.
2. No diagonal element may be zero if all elements in the row to the left of it are zero.

There is a slight chance of generating a zero diagonal element in the course of calculations. Equations which are not independent (a unique solution undefined) will also generate a zero diagonal. If it is known that the coefficient matrix is non-singular, that is, that there is a unique solution, division by zero may be easily corrected and the problem submitted again. A simple rearrangement of the columns will usually suffice. In rearranging the columns the equality vector always must be kept on the right. As indicated later, rearrangement of columns may be accomplished simply by rearranging input cards. No additional punching is required.

Tolerance Warning Level. When the diagonal element is very small relative to the values to its right in the row, a loss of accuracy will result from round-off errors. In this program the operator has control over this situation. When the absolute value of the divisor is less than or equal to some tolerance level selected by the operator, a warning message is typed. The operator then has the choice of continuing with the solution or proceeding to the next problem. If he should elect to continue, he does so with the knowledge that the answer may contain significant rounding errors. Of course, checking the answers will quickly show the accuracy of the solution.

Input Card Format

The first card of the input for each set of equations must be a card with the number of equations punched according to the FORMAT STATEMENT (I2).

The matrix of coefficients is punched column-wise beginning with the left-most column and ending with the equality column. Each column must begin with a new card. A card must contain five values punched successively according to the FORMAT STATEMENT (EL4.8). It is obvious

that the five values will take up the first 70 spaces on the card. The column may be continued over as many cards as necessary. (Five cards is the maximum number, as the program is limited to 25 unknowns.) If the number of rows is not a multiple of five, dummy zero values must be punched to finish out five entries on the last card of the column. It is never necessary to punch more than four dummy zero entries for a given column. The number of cards per column will be the same for all columns within a given problem, but may vary from problem to problem. The dummy entries used to fill out the five entries on the last card of a column need not be zero. These entries are accessed during the read in, but are never accessed during calculation. Hence they must be present, but their value is immaterial.

Output Card and Typewriter Format

The first statement for each problem will be the word SOLUTION followed by the answers typed according to FORMAT STATEMENT (El4.8). If it is desired to have the answers punched with the same format statement, Sense Switch 1 should be turned on. The word SOLUTION will not be punched; however, the answers including the word SOLUTION will continue to be typed. The cards will contain the solution, one per card in the order in which the variables appeared in the original matrix.

Sense Switch Settings

Sense Switch

1	ON	Solution is typed and punched.
	OFF	Solution is typed.
2	ON	Next problem after tolerance stop.
	OFF	Continue after tolerance stop.
3	ON	Tolerance level entered for each problem.
	OFF	Tolerance level entered only once.
4	ON	To correct error in typing tolerance level.
	OFF	Tolerance level entered correctly.

Normal Loading Procedure

1. Clear Storage
2. Depress RESET
3. Depress LOAD button
4. Depress READER START when hopper is empty
5. LOAD DATA is typed by typewriter
6. Enter data cards
7. Depress COMPUTER START
8. Depress READER START

Special Loading Instructions

At any time the program may be initialized and started by branching to 08300.

Other Instructions and Remarks

Tolerance Level. When the program begins, the typewriter will request the operator to enter the tolerance level as a floating point number in the form (+.000000).

If the entry is typed correctly, set Sense Switch 4 OFF, press RELEASE and COMPUTER START. The data cards will then be read.

If the entry is typed incorrectly, turn Sense Switch 4 ON, press RELEASE and START. The program will immediately return control to the typewriter so the entry may be made again. If the retry is correct, follow the procedure for a correct entry.

If it is desired to enter a tolerance level for each set of equations, turn Sense Switch 3 ON. If not, turn Switch 3 OFF, and the last tolerance level entered will automatically be applied to all succeeding sets of equations.

When a tolerance warning stop occurs, directions for the use of Switch 2 are typed. Only at this time is the setting of Switch 2 interrogated.

All programmed stops are accompanied by typewriter messages which are self explanatory and which indicate the required action.

SAMPLE PROBLEMS

The following four problems were used one after the other.

$$8x_1 - 5x_2 + 7x_3 = 29$$

$$+2x_2 - 2x_3 = -2$$

$$-x_1 + 9x_2 - 6x_3 = 1$$

Answer: $x_1 = 2, x_2 = 3, x_3 = 4$

$$x_1 + 2x_2 + 3x_3 - 4x_4 + 5x_5 - 6x_6 + 7x_7 - 8x_8 = -28$$

$$7x_2 \quad \quad \quad -2x_5 \quad \quad \quad + x_7 + x_8 = 19$$

$$2x_1 + 3x_2 - 4x_3 - 5x_4 \quad \quad \quad + 6x_6 \quad \quad \quad = 12$$

$$x_1 + x_2 + x_3 + x_4 + x_5 + x_6 + x_7 + x_8 = 36$$

$$10x_1 + 3x_2 - 4x_3 \quad \quad \quad + x_5 + 2x_6 - 9x_7 \quad \quad \quad = -42$$

$$3x_1 - 3x_2 - 2x_3 + 2x_4 \quad \quad \quad + x_6 \quad \quad \quad = 5$$

$$-8x_1 \quad \quad -9x_3 \quad \quad + 7x_5 \quad \quad + 6x_7 - 3x_8 = 18$$

$$\quad \quad \quad + 3x_7 - 5x_8 = -19$$

Answers: $x_1 = 1, x_2 = 2, x_3 = 3, x_4 = 4$

$x_5 = 5, x_6 = 6, x_7 = 7, x_8 = 8$

$$3x_1 + 8x_2 + 6x_3 + 10x_4 + 42x_5 = -20$$

$$+2x_2 \quad \quad + x_4 + 5x_5 = 40$$

$$+ 4x_4 + 6x_5 = -18$$

$$2x_1 + 4x_2 + 7x_3 \quad \quad + 9x_5 = 12$$

$$x_1 + 4x_2 + 6x_3 - 2x_4 + 10x_5 = 7$$

This problem will cause diagonal 3 to be zero. It was included merely to illustrate the typewriter message.

$$\begin{aligned}3x_1 + 8x_2 + 6x_3 + 10x_4 + 42x_5 &= -20 \\+ 2x_2 &\quad + x_3 + 5x_4 + 5x_5 = 40 \\+ .01x_3 + 4x_4 + 6x_5 &= -18 \\2x_1 + 4x_2 + 7x_3 &\quad + 9x_5 = 12 \\x_1 + 4x_2 + 6x_3 - 2x_4 + 10x_5 &= 7\end{aligned}$$

This problem will make diagonal 3 go below a tolerance level of 0.1. It was included merely to illustrate this typewriter message.

COMMENTS ON THE TYPEWRITER LOG

FOR SAMPLE PROBLEMS

On the typewriter log, which follows, several points should be noted. Sense Switch 3 was on at the beginning. Note that a tolerance level was entered for each of the first three problems. After the tolerance was entered for the third problem, Sense Switch 3 was turned off. When diagonal 3 went to zero and COMPUTER START was pressed to continue with the fourth problem, the solution began immediately without the entry of a tolerance level, as Switch 3 was off. Note the tolerance level in the warning message of the fourth problem is the last entry made--that for problem 3. When this warning message appeared, Switch 2 was turned off and calculation continued to obtain a solution.

490E300RS

ACCEPT TOLERANCE IN FORM +.000000 PUSH RS
+.000001RS

SOLUTION

.20000000E+01
.30000000E+01
.40000000E+01

ACCEPT TOLERANCE IN FORM +.000000 PUSH RS
+.000001RS

SOLUTION

.10000065E+01
.19999976E+01
.30000053E+01
.39999963E+01
.49999916E+01
.59999990E+01
.70000022E+01
.80000012E+01

ACCEPT TOLERANCE IN FORM +.000000 PUSH RS
+.1RS

DIAGONAL IS ZERO, PUSH START FOR NEXT PROBLEM
IS 3

DIAGONAL THAT IS LESS THAN OR EQUAL TO TOLER
IS 3

TURN SW 2 OFF TO CONT. ON FOR NEXT PROBLEM
THEN PUSH START

SOLUTION

-.67605150E+01
.34405115E+02
-.70773320E+01
.59439480E+01
-.69508359E+01

SOURCE PROGRAM FOR SOLUTION OF SIMULTANEOUS LINEAR EQUATIONS

ENTER SOURCE PROGRAM
THEN PUSH START

```

DIMENSION X(26,27)
30 FORMAT(I2)
31 FORMAT(EL4.8,EL4.8,EL4.8,EL4.8,EL4.8)
32 FORMAT(//8HSOLUTION)
33 FORMAT(44HDIAGONAL THAT IS LESS THAN OR EQUAL TO TOLER)
34 FORMAT(2HIS I3)
35 FORMAT(42HTURN SW 2 OFF TO CONT, ON FOR NEXT PROBLEM)
36 FORMAT(15HTHEN PUSH START)
37 FORMAT(45HDIAGONAL IS ZERO, PUSH START FOR NEXT PROBLEM)
38 FORMAT(41HACCEPT TOLERANCE IN FORM +.000000 PUSH RS)
39 FORMAT(F8.6)
40 FORMAT(EL4.8)
10 PRINT 38
    ACCEPT 39, TOLER
1 READ 30, N
  N1 = N + 1
  DO 2 J = 1, N1
    DO 2 I = 1, N, 5
2 READ31,X(I,J), X(I+1,J), X(I+2,J), X(I+3,J), X(I+4,J)
    DO 14 I = 1, N, 1
      DIAG = X(I,I)
      IF (DIAG) 3, 20, 4
3 IF (DIAG + TOLER) 5, 19, 19
4 IF (DIAG - TOLER) 19, 19, 5
5 DO 6 J = I, N1
6 X(I,J) = X(I,J) / DIAG
  K = 1
9 IF (K-I) 11, 13, 11
11 FELMT = X(K,I)
  DO 12 J = I, N1
12 X(K,J) = X(K,J) - FELMT * X(I,J)
13 K = K + 1
  IF (K-N) 9, 9, 14
14 CONTINUE
  J=N1
  IF (SENSe SWITCH 1) 15, 17
15 TYPE 32
  DO 16 I = 1, N
    PUNCH 40, X(I,J)
16 TYPE 40, X(I,J)
  GO TO 21
17 TYPE 32
  DO 18 I=1 , N

```

```
18 TYPE 40, X(I,J)
21 IF (SENSE SWITCH 3) 10,1
19 TYPE 33
    TYPE 34,I
    TYPE 35
    TYPE 36
    PAUSE
    IF (SENSE SWITCH 2) 21,5
20 TYPE 37
    TYPE 34,I
    PAUSE
    GO TO 21
END
```

TABLE XXX—THERMODYNAMIC PROPERTIES OF H₂ (GAS)

[Molecular weight, 2.016]

T (°K)	C _p (cal mole °K)	H ₂ —H ₂ (kcal mole)	H ₂ (kcal mole)	S _T (cal mole °K)	—ΔH° RT	+(-Δf°/RT) = -ΔT(ε/RT + δ)		log K*	δ log K = -ΔT(ε/RT + δ)	
						ε	δ		ε	δ
0	0	0	67.4169	31.2111	155.8267	71.2984
208.16	6.862**	2.6338	69.3407	31.2111	155.8267	70.7414
300	6.863	2.6345	69.3511	31.2171	154.7610	61.7421
400	6.864	2.6351	70.1479	31.2501	151.1405	46.3069
500	6.865	3.4255	70.8661	31.8070	105.4511
600	7.4408	4.1286	71.5155	36.981	88.1261	32.6649
700	7.4435	4.8315	72.2184	37.107	78.7451	27.1921
800	7.4458	5.3734	72.3513	38.108	66.4582	25.0744
900	7.4479	6.2180	73.6619	38.936	59.2322	16.8366
1000	7.4499	6.9638	74.3827	39.730	53.4175	5185	0.02306	17.2883	2291	0.03007
1100	7.4510	7.6523	75.1092	40.2071	48.7111	4772	0.02151	15.1755	2067	0.02501
1200	7.4517	8.4281	75.8150	41.045	44.7599	4318	0.02056	13.4165	110.6	0.0213
1300	7.4524	9.1730	76.3998	41.6731	41.4128	3985	0.02057	11.9135	1772	0.0192
1400	7.4535	9.9301	77.3470	42.1908	38.5100	3700	0.02051	10.6275	1648	0.0183
1500	7.4542	10.6569	78.1158	42.7227	36.0168	3454	0.02005	9.5105	1541	0.01628
1600	7.4542	11.4710	78.8009	43.2243	33.8620	3210	0.02002	8.5311	1447	0.01472
1700	7.4542	12.2613	79.6782	43.7016	31.9311	3051	0.02000	7.6552	1361	0.01392
1800	8.0185	13.0581	80.4751	44.1571	30.2121	2884	0.02001	6.8011	1260	0.01173
1900	8.1063	13.8618	81.2817	44.5610	28.7161	2734	0.02010	6.2029	1225	0.01040
2000	8.1919	14.6810	82.0669	45.0112	27.2829	2009	0.02031	5.5708	1166	0.00916
2100	8.2762	15.5036	82.9205	45.4130	26.0215	2178	0.01954	5.0151	1112	0.00865
2200	8.3571	16.3551	83.7520	45.7908	24.8786	2367	0.01867	4.5010	1063	0.00791
2300	8.4274	17.1783	84.5010	46.1728	23.8308	2267	0.01752	4.0300	1018	0.00733
2400	8.4977	18.0201	85.4373	46.5720	22.8987	2171	0.01650	3.5994	978	0.00610
2500	8.5617	18.8735	86.2854	46.8812	21.8622	2089	0.01604	3.2018	940	0.00565
2600	8.6286	19.7331	87.1500	47.2181	21.1027	2011	0.01559	2.8514	905	0.00511
2700	8.6866	20.5991	88.0160	47.5151	20.4027	1938	0.01466	2.4938	873	0.00481
2800	8.7459	21.4760	88.8878	47.8022	19.6959	1870	0.01417	2.1772	843	0.00441
2900	8.8042	22.3485	89.7551	18.1702	19.0369	1867	0.01377	1.8821	815	0.00403
3000	8.8637	23.2117	90.6186	18.4656	18.4208	1718	0.01323	1.6064	789	0.00368
3100	8.9118	24.1202	91.5371	18.7609	17.8137	1693	0.01294	1.3182	764	0.00335
3200	8.9536	25.0110	92.4309	19.0147	17.3017	1630	0.01283	1.0559	741	0.00325
3300	9.0133	25.9129	93.3298	19.3213	16.7919	1591	0.01205	.8781	719	0.00313
3400	9.0639	26.8108	94.2337	19.5911	16.3013	1516	0.01219	.6935	699	0.00279
3500	9.1125	27.7256	95.1425	19.8545	15.8574	1502	0.01208	.4610	680	0.00241
3600	9.1602	28.6392	96.0561	19.1119	15.4281	1461	0.01184	.2567	643	0.00228
3700	9.2070	29.5570	96.9745	19.3615	15.0214	1423	0.01153	.0885	614	0.00224
3800	9.2529	30.4806	97.8975	19.4977	14.6351	1386	0.01132	-.0592	628	0.00197
3900	9.2979	31.3081	98.8250	19.8206	14.2687	1351	0.01125	-.2162	613	0.00175
4000	9.3421	32.3101	99.7570	19.0866	13.9197	1318	0.01104	-.4012	598	0.00155
4100	9.3856	33.2765	100.6934	19.3178	13.5872	1287	0.01067	-.6387	584	0.00115
4200	9.4283	34.2172	101.6341	19.5145	13.2701	1257	0.01057	-.8692	571	0.00111
4300	9.4714	35.1621	102.5740	19.7055	12.9672	1229	0.01058	-.8233	558	0.00118
4400	9.5118	36.1113	103.5282	19.8750	12.6775	1201	0.01031	-.8513	540	0.00097
4500	9.5520	37.0645	104.4814	19.2162	12.4003	1175	0.01017	-.10736	533	0.00080
4600	9.5928	38.0217	105.4380	19.4066	12.1347	1150	0.01002	-1.1907	524	0.00071
4700	9.6321	38.5830	106.3999	19.6104	11.8800	1127	0.01071	-1.3029	514	0.00042
4800	9.6711	39.0182	107.3551	19.8196	11.6355	1104	0.01059	-1.4164	503	0.00045
4900	9.7069	40.0173	108.3312	19.0194	11.4005	1082	0.01030	-1.5135	494	0.00030
5000	9.7470	41.8601	109.3670	19.2150	11.1730	1061	0.01030	-1.6120	484	0.00020
5100	9.7853	42.8658	110.2837	19.4093	10.9572	1041	0.00931	-1.7077	475	0.00015
5200	9.8222	43.8472	111.2641	19.5667	10.7477	1021	0.00916	-1.7602	466	0.00018
5300	9.8580	44.8312	112.2481	19.7871	10.5554	1003	0.00881	-1.8873	458	-0.00001
5400	9.8935	45.8189	113.2358	19.9717	10.3581	985	0.00861	-1.9721	450	-0.00013
5500	9.9259	46.8101	114.2270	19.1396	10.1631	967	0.00862	-2.0359	442	-0.00013
5600	9.9619	47.8048	115.2217	19.3228	9.9516	931	0.00876	-2.1327	434	-0.00014
5700	9.9904	48.8031	116.2200	19.4065	9.8570	934	0.00867	-2.2057	427	-0.00012
5800	10.0334	49.8017	117.2216	19.4837	9.6943	919	0.00854	-2.2822	420	-0.00009
5900	10.0670	50.8007	118.2266	19.5555	9.4720	904	0.00843	-2.3531	413	-0.00008
6000	10.1001	51.8181	119.2250	19.6220	9.2420	-----	-----	-2.4216	406	-----

TABLE XLIV—THERMODYNAMIC PROPERTIES OF O₂ (GAS)

(Molecular weight, 32.0000)

T (°K.)	C _v (cal/mole °K.)	H _T -H ₀ (kcal/mole)	H _T (kcal/mole)	S _T (cal/mole °K.)	-ΔH ^a RT	$\frac{e}{R} \left(\frac{-\Delta H^a}{RT} - \frac{-\Delta T}{T^2} \left(\frac{\partial \ln K}{\partial T} + \delta \right) \right)$		log K ^b	$\delta \ln K = \frac{-\Delta T}{RT} \left(\frac{\partial \ln K}{\partial T} + \delta \right)$	
						a	b		c	d
0	0	2.0362
250	2.020	2.0737	4.1160	49.011	192.6835	80.6182
500	2.020	2.0876	4.1238	49.076	198.4695	80.6807
750	2.020	2.0977	4.8359	51.078	149.2019	58.5109
1000	2.020	2.1068	5.5650	52.728	119.7013	45.3311
1250	2.020	2.1149	6.2951	54.378	90.5650	26.8580
1500	2.020	2.1220	7.0252	55.303	82.8510	20.6499
1750	2.020	2.1284	7.8556	56.308	75.2150	25.0854
2000	2.020	2.1337	8.7060	57.327	66.9937	22.3515
2250	2.020	2.1381	9.5374	58.1900	60.3812	.0026	.02453	19.4490	.2041	.01824
2500	2.020	2.1411	10.3263	54.105	50.5650	26.8580
2750	2.020	2.1433	11.0582	55.303	48.8510	20.6499
3000	2.020	2.1455	11.8556	56.308	43.2150	25.0854
3250	2.020	2.1477	12.6160	57.327	36.9937	22.3515
3500	2.020	2.1498	13.3419	58.1900	30.3812	.0026	.02453	19.4490	.2041	.01824
3750	2.020	2.1519	14.0763	54.105	25.9650	26.8580
4000	2.020	2.1539	14.8734	55.303	22.7140	20.6499
4250	2.020	2.1559	15.5753	56.308	20.7976	15.0161	.2370	.01824
4500	2.020	2.1578	16.4610	57.327	18.6219	4.017	.01610	15.0161	.2173	.01824
4750	2.020	2.1598	17.3585	58.1900	16.4219	4.017	.01610	13.3777	.2069	.01824
5000	2.020	2.1618	18.2560	59.052	14.3015	4.017	.01610	11.9307	.1867	.01824
5250	2.020	2.1638	19.1535	59.914	12.1922	4.017	.01610	10.6732	.1744	.01824
5500	2.020	2.1657	20.0499	60.774	10.1022	4.017	.01610	9.4157	.1621	.01824
5750	2.020	2.1677	20.9464	61.6368	8.0122	4.017	.01610	8.1581	.1498	.01824
6000	2.020	2.1696	21.8429	62.5000	5.9222	4.017	.01610	6.9007	.1375	.01824
6250	2.020	2.1715	22.7394	63.3638	3.8322	4.017	.01610	5.6432	.1252	.01824
6500	2.020	2.1734	23.6359	64.2272	1.7422	4.017	.01610	4.3857	.1129	.01824
6750	2.020	2.1753	24.5334	65.0906	4.017	.01610	3.1283	.1007	.01824
7000	2.020	2.1772	25.4319	65.9541	2.0422	4.017	.01610	1.8700	.0885	.01824
7250	2.020	2.1791	26.3304	66.8176	4.017	.01610	0.6125	.0763	.01824
7500	2.020	2.1810	27.2289	67.6811	2.0422	4.017	.01610	0.3650	.0641	.01824
7750	2.020	2.1829	28.1274	68.5446	4.017	.01610	0.1175	.0519	.01824
8000	2.020	2.1848	29.0259	69.4081	2.0422	4.017	.01610	0.0000	.0397	.01824
8250	2.020	2.1867	29.9244	69.2716	4.017	.01610	0.0000	.0275	.01824
8500	2.020	2.1886	30.8229	69.1351	2.0422	4.017	.01610	0.0000	.0153	.01824
8750	2.020	2.1905	31.7214	69.9986	4.017	.01610	0.0000	.0031	.01824
9000	2.020	2.1924	32.6199	69.8621	2.0422	4.017	.01610	0.0000	.0009	.01824
9250	2.020	2.1943	33.5184	69.7256	4.017	.01610	0.0000	.0000	.01824
9500	2.020	2.1962	34.4169	69.5891	2.0422	4.017	.01610	0.0000	.0000	.01824
9750	2.020	2.1981	35.3154	69.4526	4.017	.01610	0.0000	.0000	.01824
10000	2.020	2.2000	36.2139	69.3161	2.0422	4.017	.01610	0.0000	.0000	.01824
10250	2.020	2.2019	37.1124	69.1796	4.017	.01610	0.0000	.0000	.01824
10500	2.020	2.2038	38.0109	69.0431	2.0422	4.017	.01610	0.0000	.0000	.01824
10750	2.020	2.2057	38.9094	68.9066	4.017	.01610	0.0000	.0000	.01824
11000	2.020	2.2076	39.8079	68.7701	2.0422	4.017	.01610	0.0000	.0000	.01824
11250	2.020	2.2095	40.7064	68.6336	4.017	.01610	0.0000	.0000	.01824
11500	2.020	2.2114	41.6049	68.4971	2.0422	4.017	.01610	0.0000	.0000	.01824
11750	2.020	2.2133	42.5034	68.3606	4.017	.01610	0.0000	.0000	.01824
12000	2.020	2.2152	43.4019	68.2241	2.0422	4.017	.01610	0.0000	.0000	.01824
12250	2.020	2.2171	44.3004	68.0876	4.017	.01610	0.0000	.0000	.01824
12500	2.020	2.2190	45.2089	67.9511	2.0422	4.017	.01610	0.0000	.0000	.01824
12750	2.020	2.2209	46.1074	67.8146	4.017	.01610	0.0000	.0000	.01824
13000	2.020	2.2228	47.0059	67.6781	2.0422	4.017	.01610	0.0000	.0000	.01824
13250	2.020	2.2247	47.9044	67.5416	4.017	.01610	0.0000	.0000	.01824
13500	2.020	2.2266	48.8029	67.4051	2.0422	4.017	.01610	0.0000	.0000	.01824
13750	2.020	2.2285	49.7014	67.2686	4.017	.01610	0.0000	.0000	.01824
14000	2.020	2.2304	50.6000	67.1321	2.0422	4.017	.01610	0.0000	.0000	.01824
14250	2.020	2.2323	51.4985	66.9956	4.017	.01610	0.0000	.0000	.01824
14500	2.020	2.2342	52.3970	66.8591	2.0422	4.017	.01610	0.0000	.0000	.01824
14750	2.020	2.2361	53.2955	66.7226	4.017	.01610	0.0000	.0000	.01824
15000	2.020	2.2380	54.1940	66.5861	2.0422	4.017	.01610	0.0000	.0000	.01824
15250	2.020	2.2399	55.0925	66.4506	4.017	.01610	0.0000	.0000	.01824
15500	2.020	2.2418	55.9910	66.3141	2.0422	4.017	.01610	0.0000	.0000	.01824
15750	2.020	2.2437	56.8895	66.1776	4.017	.01610	0.0000	.0000	.01824
16000	2.020	2.2456	57.7880	66.0411	2.0422	4.017	.01610	0.0000	.0000	.01824
16250	2.020	2.2475	58.6865	65.8946	4.017	.01610	0.0000	.0000	.01824
16500	2.020	2.2494	59.5850	65.7581	2.0422	4.017	.01610	0.0000	.0000	.01824
16750	2.020	2.2513	60.4835	65.6216	4.017	.01610	0.0000	.0000	.01824
17000	2.020	2.2532	61.3820	65.4851	2.0422	4.017	.01610	0.0000	.0000	.01824
17250	2.020	2.2551	62.2805	65.3486	4.017	.01610	0.0000	.0000	.01824
17500	2.020	2.2570	63.1790	65.2121	2.0422	4.017	.01610	0.0000	.0000	.01824
17750	2.020	2.2589	64.0775	65.0756	4.017	.01610	0.0000	.0000	.01824
18000	2.020	2.2608	64.9760	64.9391	2.0422	4.017	.01610	0.0000	.0000	.01824
18250	2.020	2.2627	65.8745	64.7926	4.017	.01610	0.0000	.0000	.01824
18500	2.020	2.2646	66.7730	64.6561	2.0422	4.017	.01610	0.0000	.0000	.01824
18750	2.020	2.2665	67.6715	64.5196	4.017	.01610	0.0000	.0000	.01824
19000	2.020	2.2684	68.5700	64.3831	2.0422	4.017	.01610	0.0000	.0000	.01824
19250	2.020	2.2703	69.4685	64.2466	4.017	.01610	0.0000	.0000	.01824
19500	2.020	2.2722	70.3670	64.1101	2.0422	4.017	.01610	0.0000	.0000	.01824
19750	2.020	2.2741	71.2655	63.9736	4.017	.01610	0.0000	.0000	.01824
20000	2.020	2.2760	72.1640	63.8371	2.0422	4.017	.01610	0.0000	.0000	.01824
20250	2.020	2.2779	73.0625	63.6996	4.017	.01610	0.0000	.0000	.01824
20500	2.020	2.2798	73.9610	63.5631	2.0422	4.017	.01610	0.0000	.0000	.01824
20750	2.020	2.2817	74.8595	63.4266	4.017	.01610	0.0000	.0000	.01824
21000	2.020	2.2836	75.7580	63.2891	2.0422	4.017	.01610	0.0000	.0000	.01824
21250	2.020	2.2855	76.6565	63.1526	4.017	.01610	0.0000	.0000	.01824
21500	2.020	2.2874	77.5550	62.9961	2.0422	4.017	.01610	0.0000	.0000	.01824
21750	2.020	2.2893	78.4535	62.8596	4.017	.01610	0.0000	.0000	.01824
22000	2.020	2.2912	79.3520	62.7231	2.0422	4.017	.01610	0.0000	.0000	.01824
22250	2.020	2.2931	80.2505	62.5866	4.017	.01610	0.0000	.0000	.01824
22500	2.020	2.2950	81.1490	62.4501	2.0422	4.017	.01610	0.0000	.0000	.01824
22750	2.020	2.2969	82.0475	62.3136	4.017	.01610	0.0000	.0000	.01824
23000	2.020	2.2988	82.9460	62.1771	2.0422	4.017	.01610	0.0000	.0000	.01824
23250	2.020	3.0007	83.8445	62.0406	4.017	.01610	0.0000	.0000	.01824
23500	2.020	3.0026	84.7430	61.8941	2.0422	4.017	.01610	0.0000	.0000	.01824
23750	2.020	3.0045	85.6415	61.7576	4.017	.01610	0.0000	.0000	.01824
24000	2.020	3.0064	86.5390	61.6210	2.0422	4.017	.01610	0.0000	.0000	.01824
24250	2.020	3.0083	87.4375	61.4845	4.017	.01610	0.		

GENERAL METHOD AND TABLES FOR COMPUTATION OF EQUILIBRIUM COMPOSITION AND TEMPERATURE

TABLE XXXIII—THERMODYNAMIC PROPERTIES OF H₂O (GAS)

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(Molecular weight, 18.016)

T (°K)	C _p (cal mole °K)	H _T -H ₀ (real mole)	H _T (real mole)	S _T (cal mole °K)	-ΔH° -RT	e(-ΔH°/RT) = -e(ΔH°/RT)		log K'	e log K' = -4T(e/RT+e)	
						e	s		e	s
0	0	0	0	0	0	1.000	1.000	0	0	0
208.16	8.025**	2.3677	11.3441	45.106**	370.2347	-----	-----	151.5648	-----	-----
300	8.025	2.3820	11.7331	45.151	370.0541	-----	-----	150.5708	-----	-----
400	8.035	3.1910	14.3251	47.490	273.0556	-----	-----	110.2372	-----	-----
500	8.045	4.0255	15.3566	49.344	225.9354	-----	-----	85.9609	-----	-----
600	8.055	4.8822	16.2133	50.003	187.973	-----	-----	69.7240	-----	-----
700	8.059	5.7115	17.1026	52.269	107.6663	-----	-----	58.0446	-----	-----
800	9.254	6.6856	18.0207	53.490	111.1213	-----	-----	49.3548	-----	-----
900	9.559	7.6347	18.5658	54.599	125.7485	-----	-----	42.8311	-----	-----
1000	9.804	8.6080	19.5691	55.6180	111.4355	11.015	0.07316	37.0674	4875	0.01154
1100	10.115	9.6083	20.0591	56.5712	100.3187	10.010	0.06833	32.5810	4439	0.01161
1200	10.113	10.6362	21.0673	57.4654	94.5572	6.188	0.06101	28.4309	4076	0.01162
1300	10.108	11.6662	22.0213	58.3550	87.7688	4.480	0.05137	24.6055	3704	0.01167
1400	10.109	12.7651	23.1002	59.1884	81.6758	2.780	0.04666	22.9395	3505	0.01173
1500	11.314	13.8712	25.2023	59.8687	76.4615	2.366	0.03115	20.5727	3276	0.01180
1600	11.313	14.9651	26.3262	60.5039	71.7016	6.913	0.04553	18.4983	3075	0.01184
1700	11.304	15.1089	27.4700	61.2673	67.5806	6.514	0.04101	16.6532	2908	0.01188
1800	11.708	17.3010	28.0321	61.5615	63.9267	6.160	0.03619	15.0312	2741	0.01197
1900	11.805	18.4757	29.8106	62.5887	60.6180	5.813	0.03500	13.5710	2600	0.01210
2000	12.008	19.5733	31.6044	63.2610	57.6870	5.557	0.03271	12.2533	2174	0.01217
2100	12.168	20.8806	32.2117	63.7500	55.0087	5.299	0.02966	11.0595	2150	0.01223
2200	12.256	22.1043	33.4314	64.3574	52.3704	5.064	0.02686	9.9730	2245	0.01227
2300	12.364	23.3313	34.6623	64.9045	50.3418	4.816	0.02468	8.9708	2160	0.01230
2400	12.463	24.5727	35.4638	65.4528	48.267	4.623	0.02230	8.0534	2072	0.01240
2500	12.551	25.8245	37.1546	65.9344	46.1333	4.471	0.02049	7.2289	1991	0.01243
2600	12.638	27.0831	38.4142	66.4274	44.0732	4.304	0.01863	6.4532	1916	0.01247
2700	12.715	28.3508	39.6819	66.9150	43.0665	4.149	0.01711	5.7443	1816	0.01256
2800	12.786	29.6258	40.9560	67.3766	41.5618	4.045	0.01577	5.0751	1751	0.01265
2900	12.852	30.9677	42.2088	67.8294	40.1633	3.871	0.01407	4.4334	1721	0.01273
3000	12.913	32.1650	43.5271	68.2661	38.8409	3.747	0.01239	3.8617	1666	0.01278
3100	12.968	33.4960	44.8211	68.6504	37.6298	3.630	0.01113	3.3170	1613	0.01284
3200	13.018	34.7893	46.1204	69.1629	36.4943	3.529	0.00955	2.8100	1575	0.01295
3300	13.064	36.0634	47.4245	69.5612	35.4177	3.417	0.00860	2.3255	1520	0.01312
3400	13.107	37.1020	48.7301	69.8919	34.4038	3.310	0.00753	1.8729	1473	0.01324
3500	13.147	38.7147	50.0458	70.2754	33.4473	3.218	0.00673	1.4458	1431	0.01330
3600	13.184	40.0612	51.3623	70.6663	32.5136	3.112	0.00561	1.0422	1392	0.01338
3700	13.218	41.3534	52.6821	71.0800	31.6884	3.019	0.00556	0.6301	1355	0.01352
3800	13.250	42.6747	54.0055	71.3609	30.8779	2.951	0.00484	2.2678	1320	0.01354
3900	13.280	43.0112	55.3221	71.5034	30.1087	2.897	0.00425	0.1042	1287	0.01358
4000	13.308	45.3366	56.6617	72.0420	29.3777	2.836	0.00370	-0.3732	1245	0.01360
4100	13.334	46.6627	57.9633	72.3710	28.6822	2.769	0.00321	-0.6843	1216	0.01440
4200	13.358	47.9973	59.3284	72.6226	28.0197	2.705	0.00283	-0.8812	1198	0.01449
4300	13.381	50.3343	60.6554	73.0471	27.3875	2.643	0.00252	-1.2643	1179	0.01449
4400	13.403	52.7252	62.0360	73.3150	26.7845	2.584	0.00228	-1.5347	1144	0.01438
4500	13.424	53.0148	63.3459	73.6164	26.2079	2.524	0.00204	-1.7933	1119	0.01434
4600	13.44	53.2582	64.6803	73.9117	25.6533	2.473	0.00193	-2.0409	1095	0.01412
4700	13.464	54.7636	66.0347	74.2011	25.1281	2.421	0.00193	-2.2750	1073	0.01396
4800	13.481	56.0510	67.3821	74.4847	24.6218	2.371	0.00183	-2.4765	1051	0.01381
4900	13.502	57.3602	68.7215	75.1463	24.1361	2.323	0.00170	-2.7346	1030	0.01370
5000	13.521	58.7114	70.0825	75.6559	23.6998	2.276	0.00163	-2.9435	1010	0.01364
5100	13.540	60.1045	71.4555	76.3058	23.2217	2.232	0.00177	-3.1351	991	0.01342
5200	13.559	61.4564	72.7065	75.5650	22.7037	2.184	0.00168	-3.3231	973	0.01322
5300	13.577	62.8162	74.1473	75.8254	22.3766	2.138	0.00172	-3.5159	953	0.01314
5400	13.596	64.1748	75.0659	76.0764	21.9743	2.088	0.00163	-3.7240	936	0.01305
5500	13.614	65.3553	76.8604	76.3550	21.5916	2.030	0.00160	-3.9245	921	0.01304
5600	13.631	66.8977	78.2288	76.5745	21.2203	2.003	0.00163	-4.0370	905	0.01293
5700	13.651	68.2619	79.5650	76.8130	20.8620	1.986	0.00162	-4.1887	890	0.01285
5800	13.669	69.6279	80.9560	77.0635	20.5139	1.963	0.00160	-4.3350	875	0.01279
5900	13.687	70.9657	82.3268	77.2673	20.1816	1.940	0.00163	-4.4981	860	0.01277
6000	13.703	72.3683	83.6844	77.4575	19.8563	-----	-----	-4.6482	850	0.01274

GENERAL METHOD AND TABLES FOR COMPUTATION OF EQUILIBRIUM COMPOSITION AND TEMPERATURE

TABLE XLIII—THERMODYNAMIC PROPERTIES OF O₂ (GAS)

[Atomic weight, 16.0000]

T (°K)	C ₂ (cal 1000 °K)	H ₂ - H ₁ (kcal mole)	H ₁ (kcal mole)	S ₂ (cal mole °K)
0	0	30.0001
200	5.2261	1.0074	31.2175	32.4000
300	5.2339	1.6170	31.2211	32.3610
400	5.1511	2.1319	31.7300	30.9915
500	5.0802	2.6154	32.2495	31.1908
600	5.0486	3.1317	32.7338	32.0540
700	5.0251	3.6535	33.2506	32.6307
800	5.0150	4.1576	33.7617	33.3011
900	5.0055	4.6587	34.2628	34.0914
1000	4.9988	5.1588	34.7639	34.6181
1100	4.9936	5.6584	35.2625	35.0945
1200	4.9894	6.1576	35.7617	35.5286
1300	4.9864	6.6564	36.2605	35.9281
1400	4.9838	7.1519	36.7600	36.2997
1500	4.9819	7.6552	37.2673	36.6113
1600	4.9805	8.1513	37.7555	36.9128
1700	4.9792	8.6494	38.2334	37.2016
1800	4.9781	9.1471	38.7512	37.4932
1900	4.9778	9.6450	39.2191	37.8184
2000	4.9776	10.1427	39.7468	38.0747
2100	4.9778	10.6405	40.2446	38.3165
2200	4.9784	11.1384	40.7424	38.5181
2300	4.9796	11.6362	41.2403	38.7157
2400	4.9812	12.1343	41.7381	38.8814
2500	4.9834	12.6325	42.2366	39.1818
2600	4.9862	13.1310	42.7351	39.3803
2700	4.9897	13.6288	43.2339	39.5800
2800	4.9935	14.1269	43.7330	39.7801
2900	4.9966	14.6255	44.2326	39.9254
3000	5.0041	15.1247	44.7328	40.0650
3100	5.0102	15.6234	45.2335	40.2592
3200	5.0170	16.1221	45.7338	40.4185
3300	5.0245	16.6218	46.2339	40.5728
3400	5.0325	17.1217	46.7338	40.7229
3500	5.0411	17.6303	47.2334	40.8689
3600	5.0502	18.1390	47.7480	41.0111
3700	5.0599	18.6484	48.2335	41.1496
3800	5.0700	19.1580	48.7600	41.2846
3900	5.0805	19.6681	49.2675	41.4165
4000	5.0914	20.1780	49.7761	41.5452
4100	5.1026	20.6877	50.2858	41.6711
4200	5.1140	21.1965	50.7966	41.7942
4300	5.1257	21.7055	51.3086	41.9147
4400	5.1375	22.2157	51.8218	42.0325
4500	5.1495	22.7250	52.3361	42.1483
4600	5.1616	23.2376	52.8517	42.2615
4700	5.1738	23.7494	53.3665	42.3727
4800	5.1860	24.2624	53.8865	42.4817
4900	5.1981	24.8016	54.4057	42.5888
5000	5.2102	25.3220	54.9261	42.6939
5100	5.2223	25.8436	55.4477	42.7973
5200	5.2344	26.3644	55.9705	42.8988
5300	5.2464	26.8855	56.4945	42.9966
5400	5.2583	27.4157	57.0188	43.0933
5500	5.2701	27.9421	57.5462	43.1943
5600	5.2818	28.4697	58.0738	43.2864
5700	5.2933	28.9965	58.6026	43.3820
5800	5.3047	29.5294	59.1323	43.4742
5900	5.3165	30.0624	59.6625	43.5649
6000	5.3279	30.6016	60.1987	43.6644

GENERAL METHOD AND TABLES FOR COMPUTATION OF EQUILIBRIUM COMPOSITION AND PERCOLATION

TABLE XXIX—THERMODYNAMIC PROPERTIES OF H (GAS)

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[Atomic weight, 1.008]

T (°K)	C_p (cal mole°K)	$H_f^o - H_f^o$ (kcal mole)	S_f^o (kcal mole)	S_f^o (cal mole°K)
0	4.0080	0	45.3245	37.3927
298.16	4.0080	1.4512	46.6797	37.3927
300	4.0080	1.4504	46.6189	37.4233
400	4.0080	1.9872	57.3157	38.8524
500	4.0080	2.4810	67.8125	39.6010
600	4.0080	2.9508	68.3093	39.8507
700	4.0080	3.4276	68.8061	39.9325
800	4.0080	3.9511	69.3029	39.2050
900	4.0080	4.4712	69.7167	39.8811
1000	4.0080	4.9880	69.2003	39.4045
1100	4.0080	5.4948	69.7033	39.8780
1200	4.0080	5.9916	69.2001	39.3103
1300	4.0080	6.4881	69.7869	39.7079
1400	4.0080	6.9852	69.2837	39.0761
1500	4.0080	7.4720	69.7805	39.4188
1600	4.0080	7.9588	69.2773	39.7305
1700	4.0080	8.4456	69.7741	39.0407
1800	4.0080	8.9324	69.2709	39.3216
1900	4.0080	9.4192	69.7677	39.5932
2000	4.0080	9.8059	69.2645	39.8480
2100	4.0080	10.4728	69.7613	39.0004
2200	4.0080	10.9246	69.2581	39.3215
2300	4.0080	11.4261	69.7549	39.5124
2400	4.0080	11.9232	69.2517	39.7538
2500	4.0080	12.4200	69.7485	39.0566
2600	4.0080	12.9168	69.2453	39.1515
2700	4.0080	13.4135	69.7421	39.3310
2800	4.0080	13.9104	69.2389	39.5106
2900	4.0080	14.4072	69.7357	39.6910
3000	4.0080	14.9040	69.2325	39.8624
3100	4.0080	15.4008	69.7293	39.0253
3200	4.0080	15.8976	69.2261	39.1830
3300	4.0080	16.3944	69.7229	39.3359
3400	4.0080	16.8912	69.2197	39.4842
3500	4.0080	17.3880	69.7165	39.6282
3600	4.0080	17.8848	69.2133	39.7681
3700	4.0080	18.3816	69.7101	39.9043
3800	4.0080	18.8784	69.2069	40.0318
3900	4.0080	19.3752	69.7037	40.1624
4000	4.0080	19.8720	69.2005	40.2916
4100	4.0080	20.3688	69.6973	40.4142
4200	4.0080	20.8656	69.1941	40.5340
4300	4.0080	21.3624	69.6909	40.6509
4400	4.0080	21.8592	69.1877	40.7851
4500	4.0080	22.3570	69.6845	40.8767
4600	4.0080	22.8538	69.1813	40.9559
4700	4.0080	23.3506	69.6781	41.0325
4800	4.0080	23.8474	69.1749	41.1073
4900	4.0080	24.3442	69.6717	41.2008
5000	4.0080	24.8410	69.1685	41.4002
5100	4.0080	25.3378	69.6653	41.4985
5200	4.0080	25.8346	69.1621	41.5950
5300	4.0080	26.3314	69.6589	41.6903
5400	4.0080	26.8282	69.1557	41.7825
5500	4.0080	27.3250	69.6525	41.8738
5600	4.0080	27.8218	69.1493	41.9632
5700	4.0080	28.3176	69.6461	42.0511
5800	4.0080	28.8144	69.1429	42.1376
5900	4.0080	29.3112	69.6397	42.2204
6000	4.0080	29.8080	69.1365	42.3059

GENERAL METHOD AND TABLES FOR COMPUTATION OF EQUILIBRIUM COMPOSITION AND TEMPERATURE

TABLE XLV—THERMODYNAMIC PROPERTIES OF OH (GAS)

[Molecular weight, 17.008]

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T °K.	C_p (cal/mole °K.)	$H_f - H_f^0$ (kcal/mole)	H_f^0 (kcal/mole)	N_p (mole/K.)	$-\frac{\Delta H^\circ}{RT}$	$\log \frac{(-\Delta H^\circ)}{RT} - \frac{-\delta T}{100} \left(\frac{e}{T^{1+\delta}} \right)$	$k \times K$	$\delta \log K = \frac{-\delta T}{100} \left(\frac{e}{T^{1+\delta}} \right)$	
						e	d		
200	7.141	0	41.7206	43.888	116.2827
200	7.141	21.002	46.8428	43.931	116.3016	68.3677
200	7.141	21.1225	46.8430	43.931	116.3016	68.3610
200	7.141	21.2426	46.8432	43.931	116.3016	20.4505
200	7.141	21.3627	46.8434	43.931	116.3016	38.3522
200	7.141	21.4828	46.8436	43.931	116.3016
200	7.141	21.6029	46.8438	43.931	116.3016
200	7.141	21.7230	46.8440	43.931	116.3016
200	7.141	21.8431	46.8442	43.931	116.3016
200	7.141	21.9632	46.8444	43.931	116.3016
200	7.141	22.0833	46.8446	43.931	116.3016
200	7.141	22.2034	46.8448	43.931	116.3016
200	7.141	22.3235	46.8450	43.931	116.3016
200	7.141	22.4436	46.8452	43.931	116.3016
200	7.141	22.5637	46.8454	43.931	116.3016
200	7.141	22.6838	46.8456	43.931	116.3016
200	7.141	22.8039	46.8458	43.931	116.3016
200	7.141	22.9240	46.8460	43.931	116.3016
200	7.141	23.0441	46.8462	43.931	116.3016
200	7.141	23.1642	46.8464	43.931	116.3016	14.9267	2029
200	7.141	23.2843	46.8466	43.931	116.3016	14.9215	0.02157
200	7.141	23.4044	46.8468	43.931	116.3016	14.9153	0.02172
200	7.141	23.5245	46.8470	43.931	116.3016	14.9093	0.02140
200	7.141	23.6446	46.8472	43.931	116.3016	14.9033	0.02167
200	7.141	23.7647	46.8474	43.931	116.3016	14.8971	0.02184
200	7.141	23.8848	46.8476	43.931	116.3016	14.8909	0.02201
200	7.141	24.0049	46.8478	43.931	116.3016	2227	0.02221
200	7.141	24.1250	46.8480	43.931	116.3016
200	7.141	24.2451	46.8482	43.931	116.3016
200	7.141	24.3652	46.8484	43.931	116.3016
200	7.141	24.4853	46.8486	43.931	116.3016
200	7.141	24.6054	46.8488	43.931	116.3016
200	7.141	24.7255	46.8490	43.931	116.3016
200	7.141	24.8456	46.8492	43.931	116.3016
200	7.141	24.9657	46.8494	43.931	116.3016
200	7.141	25.0858	46.8496	43.931	116.3016
200	7.141	25.2059	46.8498	43.931	116.3016
200	7.141	25.3260	46.8500	43.931	116.3016
200	7.141	25.4461	46.8502	43.931	116.3016
200	7.141	25.5662	46.8504	43.931	116.3016
200	7.141	25.6863	46.8506	43.931	116.3016
200	7.141	25.8064	46.8508	43.931	116.3016
200	7.141	25.9265	46.8510	43.931	116.3016
200	7.141	26.0466	46.8512	43.931	116.3016
200	7.141	26.1667	46.8514	43.931	116.3016
200	7.141	26.2868	46.8516	43.931	116.3016
200	7.141	26.4069	46.8518	43.931	116.3016
200	7.141	26.5270	46.8520	43.931	116.3016
200	7.141	26.6471	46.8522	43.931	116.3016
200	7.141	26.7672	46.8524	43.931	116.3016
200	7.141	26.8873	46.8526	43.931	116.3016
200	7.141	27.0074	46.8528	43.931	116.3016
200	7.141	27.1275	46.8530	43.931	116.3016
200	7.141	27.2476	46.8532	43.931	116.3016
200	7.141	27.3677	46.8534	43.931	116.3016
200	7.141	27.4878	46.8536	43.931	116.3016
200	7.141	27.6079	46.8538	43.931	116.3016
200	7.141	27.7280	46.8540	43.931	116.3016
200	7.141	27.8481	46.8542	43.931	116.3016
200	7.141	27.9682	46.8544	43.931	116.3016
200	7.141	28.0883	46.8546	43.931	116.3016
200	7.141	28.2084	46.8548	43.931	116.3016
200	7.141	28.3285	46.8550	43.931	116.3016
200	7.141	28.4486	46.8552	43.931	116.3016
200	7.141	28.5687	46.8554	43.931	116.3016
200	7.141	28.6888	46.8556	43.931	116.3016
200	7.141	28.8089	46.8558	43.931	116.3016
200	7.141	28.9290	46.8560	43.931	116.3016
200	7.141	29.0491	46.8562	43.931	116.3016
200	7.141	29.1692	46.8564	43.931	116.3016
200	7.141	29.2893	46.8566	43.931	116.3016
200	7.141	29.4094	46.8568	43.931	116.3016
200	7.141	29.5295	46.8570	43.931	116.3016
200	7.141	29.6496	46.8572	43.931	116.3016
200	7.141	29.7697	46.8574	43.931	116.3016
200	7.141	29.8898	46.8576	43.931	116.3016
200	7.141	30.0099	46.8578	43.931	116.3016
200	7.141	30.1299	46.8580	43.931	116.3016
200	7.141	30.2499	46.8582	43.931	116.3016
200	7.141	30.3699	46.8584	43.931	116.3016
200	7.141	30.4899	46.8586	43.931	116.3016
200	7.141	30.6099	46.8588	43.931	116.3016
200	7.141	30.7299	46.8590	43.931	116.3016
200	7.141	30.8499	46.8592	43.931	116.3016
200	7.141	30.9699	46.8594	43.931	116.3016
200	7.141	31.0899	46.8596	43.931	116.3016
200	7.141	31.2099	46.8598	43.931	116.3016
200	7.141	31.3299	46.8600	43.931	116.3016
200	7.141	31.4499	46.8602	43.931	116.3016
200	7.141	31.5699	46.8604	43.931	116.3016
200	7.141	31.6899	46.8606	43.931	116.3016
200	7.141	31.8099	46.8608	43.931	116.3016
200	7.141	31.9299	46.8610	43.931	116.3016
200	7.141	32.0499	46.8612	43.931	116.3016
200	7.141	32.1699	46.8614	43.931	116.3016
200	7.141	32.2899	46.8616	43.931	116.3016
200	7.141	32.4099	46.8618	43.931	116.3016
200	7.141	32.5299	46.8620	43.931	116.3016
200	7.141	32.6499	46.8622	43.931	116.3016
200	7.141	32.7699	46.8624	43.931	116.3016
200	7.141	32.8899	46.8626	43.931	116.3016
200	7.141	33.0099	46.8628	43.931	116.3016
200	7.141	33.1299	46.8630	43.931	116.3016
200	7.141	33.2499	46.8632	43.931	116.3016
200	7.141	33.3699	46.8634	43.931	116.3016
200	7.141	33.4899	46.8636	43.931	116.3016
200	7.141	33.6099	46.8638	43.931	116.3016
200	7.141	33.7299	46.8640	43.931	116.3016
200	7.141	33.8499	46.8642	43.931	116.3016
200	7.141	33.9699	46.8644	43.931	116.3016
200	7.141	34.0899	46.8646	43.931	116.3016
200	7.141	34.2099	46.8648	43.931	116.3016
200	7.141	34.3299	46.8650	43.931	116.3016
200	7.141	34.4499	46.8652	43.931	116.3016
200	7.141	34.5699	46.8654	43.931	116.3016
200	7.141	34.6899	46.8656	43.931	116.3016
200	7.141	34.8099	46.8658	43.931	116.3016
200	7.141	34.9299	46.8660	43.931	116.3016
200	7.141	35.0499	46.8662	43.931	116.3016
200	7.141	35.1699	46.8664</td						